

=> file registry

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STRUCTURE FILE UPDATES: 27 SEP 2007 HIGHEST RN 948530-59-4
 DICTIONARY FILE UPDATES: 27 SEP 2007 HIGHEST RN 948530-59-4

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=> file zcaplus

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FILE COVERS 1907 - 28 Sep 2007 VOL 147 ISS 15
 FILE LAST UPDATED: 27 Sep 2007 (20070927/ED)

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 substance identification.

'OBI' IS DEFAULT SEARCH FIELD FOR 'ZCAPLUS' FILE

=> d stat que L55

| | | | | | | |
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| L3 | 1 | SEA | FILE=REGISTRY | ABB=ON | PLU=ON | 192126-76-4 |
| L5 | 1 | SEA | FILE=REGISTRY | ABB=ON | PLU=ON | 709044-44-0 |
| L6 | 1 | SEA | FILE=REGISTRY | ABB=ON | PLU=ON | 847493-45-2 |
| L8 | 1 | SEA | FILE=REGISTRY | ABB=ON | PLU=ON | 6088-50-2 |
| L9 | 1 | SEA | FILE=REGISTRY | ABB=ON | PLU=ON | 105988-28-1 |
| L10 | 1 | SEA | FILE=REGISTRY | ABB=ON | PLU=ON | 847493-44-1 |

L11 1 SEA FILE=REGISTRY ABB=ON PLU=ON 847493-46-3
 L13 26734 SEA FILE=ZCAPLUS ABB=ON PLU=ON THIOLS+OLD/CT
 L14 264757 SEA FILE=ZCAPLUS ABB=ON PLU=ON PUR/RL
 L15 32 SEA FILE=ZCAPLUS ABB=ON PLU=ON L13 (L) L14
 L16 118162 SEA FILE=ZCAPLUS ABB=ON PLU=ON DISULFID?/BI
 L17 147 SEA FILE=ZCAPLUS ABB=ON PLU=ON DI SULFID?/BI
 L18 1626 SEA FILE=ZCAPLUS ABB=ON PLU=ON BISULFID?/BI OR BI SULFID?/BI

 L19 11 SEA FILE=ZCAPLUS ABB=ON PLU=ON L15 AND (L16 OR L17 OR L18)
 L24 120255 SEA FILE=ZCAPLUS ABB=ON PLU=ON ?DISULFID?/BI
 L25 167140 SEA FILE=ZCAPLUS ABB=ON PLU=ON ?THIOL?/BI
 L26 20268 SEA FILE=ZCAPLUS ABB=ON PLU=ON L24 AND L25
 L31 14 SEA FILE=ZCAPLUS ABB=ON PLU=ON (L3 OR L5 OR L6 OR (L8 OR L9
 OR L10 OR L11)) AND L26
 L32 4 SEA FILE=ZCAPLUS ABB=ON PLU=ON L19 AND 75-15-0?/OBI
 L33 7 SEA FILE=ZCAPLUS ABB=ON PLU=ON L19 NOT L32
 L35 2 SEA FILE=ZCAPLUS ABB=ON PLU=ON L31 AND ?ISOLAT?/OBI
 L36 1 SEA FILE=ZCAPLUS ABB=ON PLU=ON L31 AND TOTAL/TI
 L37 1 SEA FILE=ZCAPLUS ABB=ON PLU=ON L31 AND REDUCTION?/TI
 L52 10 SEA FILE=ZCAPLUS ABB=ON PLU=ON L33 OR (L35 OR L36 OR L37)
 L54 60 SEA FILE=ZCAPLUS ABB=ON PLU=ON STEENKAMP D?/AU
 L55 2 SEA FILE=ZCAPLUS ABB=ON PLU=ON L52 AND L54

=> d stat que L56

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 L28 1351 SEA FILE=ZCAPLUS ABB=ON PLU=ON L26 AND L27
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 L56 3 SEA FILE=ZCAPLUS ABB=ON PLU=ON L28 AND L54

=> s L55 or L56

L93 3 L55 OR L56

=> d ibib abs hitind hitstr L93 1-3

L93 ANSWER 1 OF 3 ZCAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 2005:216793 ZCAPLUS Full-text
 DOCUMENT NUMBER: 142:278860
 TITLE: A method of *isolating a thiol*
 INVENTOR(S): **Steenkamp, Daniel Jacobus**
 PATENT ASSIGNEE(S): University of Cape Town, S. Afr.
 SOURCE: PCT Int. Appl., 26 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---------------|---|----------|-----------------|----------|
| ----- | ---- | ----- | ----- | ----- |
| WO 2005021493 | A2 | 20050310 | WO 2004-IB2774 | 20040827 |
| WO 2005021493 | A3 | 20050414 | | |
| W: | AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, | | | |

NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY,
 TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
 RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM,
 AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK,
 EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE,
 SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE,
 SN, TD, TG

PRIORITY APPLN. INFO.:

ZA 2003-6684

A 20030827

OTHER SOURCE(S): MARPAT 142:278860

AB The invention relates to a method of isolating a **thiol** R'SH from a **thiol** containing mixture. The method includes the steps of forming a mixed **disulfide** R'SSR of the **thiol** R'SH, **purifying** the mixed **disulfide** R'SSR and reducing the **purified** mixed **disulfide** R'SSR. The **thiol** R'SH is thereafter isolated. The invention extends to a **disulfide** of the formula R'SSR.

IC ICM C07C381-00

CC 16-1 (Fermentation and Bioindustrial Chemistry)

ST **thiol purifn** fermn **disulfide** deriv

IT Fermentation

Mycobacterium smegmatis

(isolating a **thiol** from fermentation)IT **Thiols, preparation**

RL: BMF (Bioindustrial manufacture); **PUR (Purification or recovery)**; RCT (Reactant); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)

(isolating a **thiol** from fermentation)IT **192126-76-4P, Mycothiol**

RL: BMF (Bioindustrial manufacture); **PUR (Purification or recovery)**; RCT (Reactant); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)

(isolating a **thiol** from fermentation)

IT 3483-12-3, Dithiothreitol

RL: NUU (Other use, unclassified); RCT (Reactant); RACT (Reactant or reagent); USES (Uses)

(isolating a **thiol** from fermentation)IT **709044-44-OP 847493-45-2P, 2-S-Mycothioly****-6-hydroxynaphthalene disulfide**

RL: **PUR (Purification or recovery)**; RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(isolating a **thiol** from fermentation)IT 70-18-8, Glutathione, reactions **6088-50-2 105988-28-1,****2-Pyridinesulfenothioic acid 847493-44-1**

RL: RCT (Reactant); RACT (Reactant or reagent)

(isolating a **thiol** from fermentation)IT **847493-46-3P, 2-S-Glutathionyl-6-hydroxynaphthalene disulfide**

RL: SPN (Synthetic preparation); PREP (Preparation)

(isolating a **thiol** from fermentation)IT **192126-76-4P, Mycothiol**

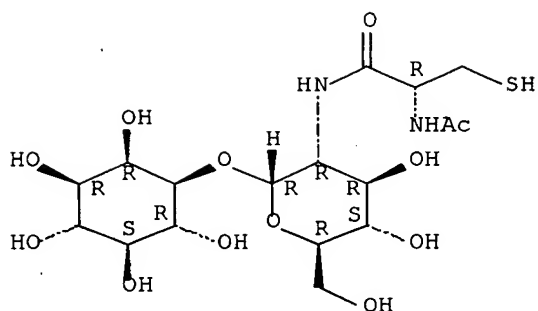
RL: BMF (Bioindustrial manufacture); **PUR (Purification or recovery)**; RCT (Reactant); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)

(isolating a **thiol** from fermentation)

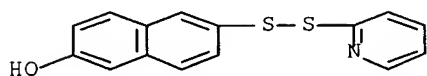
RN 192126-76-4 ZCAPLUS

CN D-myo-Inositol, 1-O-[2-[[(2R)-2-(acetylamino)-3-mercapto-1-oxopropyl]amino]-2-deoxy- α -D-glucopyranosyl]- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

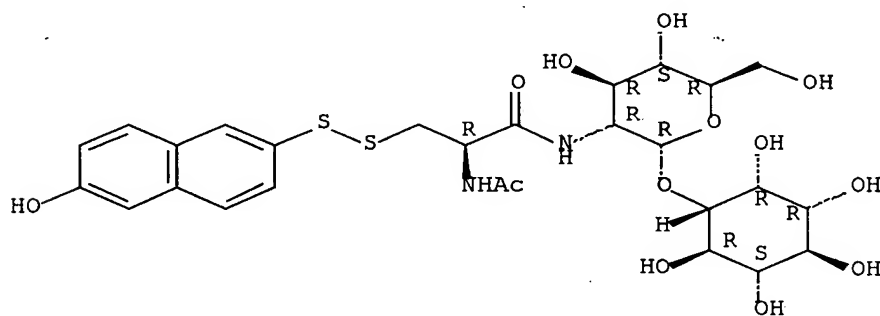


IT 709044-44-0P 847493-45-2P, 2-S-Mycothioly
 -6-hydroxynaphthalene **disulfide**.
 RL: PUR (Purification or recovery); RCT (Reactant); SPN (Synthetic
 preparation); PREP (Preparation); RACT (Reactant or reagent)
 (**isolating** a **thiol** from fermentation)
 RN 709044-44-0 ZCAPLUS
 CN 2-Naphthalenol, 6-(2-pyridinyldithio)- (9CI) (CA INDEX NAME)

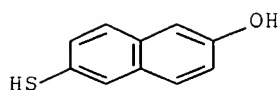


RN 847493-45-2 ZCAPLUS
 CN D-myo-Inositol, 1-O-[2-[[(2R)-2-(acetylamino)-3-[(6-hydroxy-2-
 naphthalenyl)dithio]-1-oxopropyl]amino]-2-deoxy- α -D-glucopyranosyl]-
 (9CI) (CA INDEX NAME)

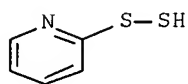
Absolute stereochemistry.



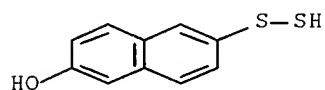
IT 6088-50-2 105988-28-1, 2-Pyridinesulfenothioic acid
 847493-44-1
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (**isolating** a **thiol** from fermentation)
 RN 6088-50-2 ZCAPLUS
 CN 2-Naphthalenol, 6-mercapto- (9CI) (CA INDEX NAME)



RN 105988-28-1 ZCAPLUS
 CN 2-Pyridinesulfenothioic acid (9CI) (CA INDEX NAME)

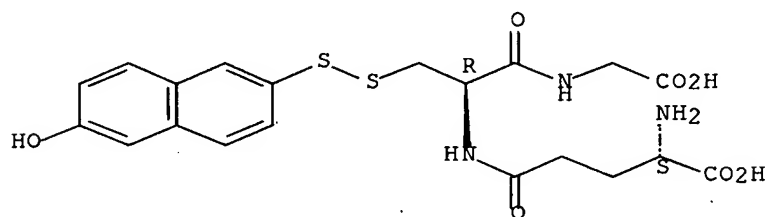


RN 847493-44-1 ZCAPLUS
 CN 2-Naphthalenesulfenothioic acid, 6-hydroxy- (CA INDEX NAME)



IT **847493-46-3P**, 2-S-Glutathionyl-6-hydroxynaphthalene
disulfide
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (**isolating** a **thiol** from fermentation)
 RN 847493-46-3 ZCAPLUS
 CN Glycine, L-γ-glutamyl-3-[(6-hydroxy-2-naphthalenyl)dithio]-L-alanyl-
 (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L93 ANSWER 2 OF 3 ZCAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 2004:30260 ZCAPLUS Full-text
 DOCUMENT NUMBER: 141:50006
 TITLE: Preparation and utilization of a reagent for the
isolation and **purification** of
 low-molecular-mass **thiols**
 AUTHOR(S): **Steenkamp, Daniel J.**; Vogt, Ryan N.

CORPORATE SOURCE: Faculty of Health Sciences, Division of Chemical Pathology, University of Cape Town, Cape Town, 7935, S. Afr.
 SOURCE: Analytical Biochemistry (2004), 325(1), 21-27
 CODEN: ANBCA2; ISSN: 0003-2697
 PUBLISHER: Elsevier Science
 DOCUMENT TYPE: Journal
 LANGUAGE: English

AB Problems inherent in the isolation of **thiols** from natural sources, such as oxidation, undesirable addition reactions, and low concentration of **thiol** species in cell-free exts., can be circumvented by reversible derivatization to a less labile form which can be concentrated selectively. These objectives are realized by converting **thiols** to **heterodisulfides** in which the **thiol** partner is an apolar **thiol** with strong affinity for hydrophobic stationary phases. When reacted with 2-S-(2'-thiopyridyl)-6- **hydroxynaphthyl**disulfide at pH<5, where most **thiol** species are relatively stable to atmospheric oxidation, mixed **disulfides** with 2-mercapto-6-hydroxynaphthalene as the apolar partner are obtained in good yield and can be concentrated onto a hydrophobic stationary phase. Such **heterodisulfides** exhibit excellent chromatog. properties when separated on reversed-phase media and the derivatization reaction can, therefore, be conveniently monitored. Following their isolation as the **heterodisulfides** the **thiol** species of interest are recovered by reduction and facile separation from the apolar 2-mercapto-6-hydroxynaphthalene partner.

CC 9-15 (Biochemical Methods)
 Section cross-reference(s): 80

ST reagent **thiol** thiopyridyl **hydroxynaphthyl**disulfide
mycothiol glutathione glutathionylspermidine redn oxidn

IT Oxidation
 Reduction
 (preparation and utilization of reagent for **isolation** and **purification** of low-mol.-mass **thiols** from biol. system)

IT 70-18-8, Glutathione, analysis 3483-12-3, DTT 33932-35-3, Glutathionylspermidine **192126-76-4, Mycothiol**
 RL: ANT (Analyte); BSU (Biological study, unclassified); ANST (Analytical study); BIOL (Biological study)
 (preparation and utilization of reagent for **isolation** and **purification** of low-mol.-mass **thiols** from biol. system)

IT **709044-44-0**
 RL: ARG (Analytical reagent use); BSU (Biological study, unclassified); ANST (Analytical study); BIOL (Biological study); USES (Uses)
 (preparation and utilization of reagent for **isolation** and **purification** of low-mol.-mass **thiols** from biol. system)

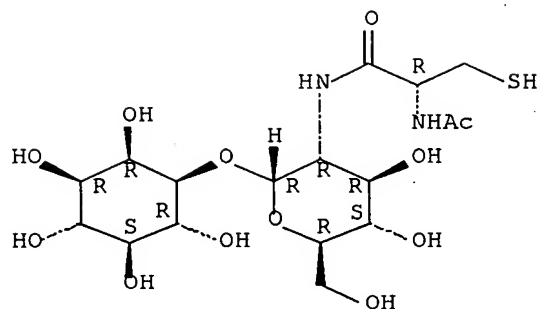
IT **6088-50-2**
 RL: BSU (Biological study, unclassified); BIOL (Biological study)
 (preparation and utilization of reagent for **isolation** and **purification** of low-mol.-mass **thiols** from biol. system)

IT **192126-76-4, Mycothiol**
 RL: ANT (Analyte); BSU (Biological study, unclassified); ANST (Analytical study); BIOL (Biological study)
 (preparation and utilization of reagent for **isolation** and **purification** of low-mol.-mass **thiols** from biol. system)

RN 192126-76-4 ZCAPLUS

CN D-myo-Inositol, 1-O-[2-[[(2R)-2-(acetylamino)-3-mercapto-1-oxopropyl]amino]-2-deoxy- α -D-glucopyranosyl]- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

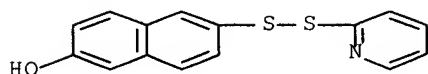


IT 709044-44-0

RL: ARG (Analytical reagent use); BSU (Biological study, unclassified);
ANST (Analytical study); BIOL (Biological study); USES (Uses)
(preparation and utilization of reagent for **isolation** and
purification of low-mol.-mass **thiols** from biol. system)

RN 709044-44-0 ZCAPLUS

CN 2-Naphthalenol, 6-(2-pyridinyldithio)- (9CI) (CA INDEX NAME)

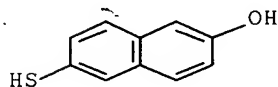


IT 6088-50-2

RL: BSU (Biological study, unclassified); BIOL (Biological study)
(preparation and utilization of reagent for **isolation** and
purification of low-mol.-mass **thiols** from biol. system)

RN 6088-50-2 ZCAPLUS

CN 2-Naphthalenol, 6-mercapto- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L93 ANSWER 3 OF 3 ZCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1994:529567 ZCAPLUS Full-text

DOCUMENT NUMBER: 121:129567

TITLE: Identification of a major low-molecular-mass
thiol of the trypanosomatid *Crithidia*
fasciculata as **ovothiol** A. Facile isolation
and structural analysis of the bimane derivative

AUTHOR(S): **Steenkamp, Daniel J.**; Spies, Hendrik S. C.

CORPORATE SOURCE: Med. Sch., Univ. Cape Town, S. Afr.

SOURCE: European Journal of Biochemistry (1994), 223(1), 43-50
CODEN: EJBCAI; ISSN: 0014-2956

DOCUMENT TYPE: Journal

LANGUAGE: English

- AB An unidentified low-mol.-mass **thiol**, U23, previously detected as the 7-diethylamino-3-(4'-maleimidylphenyl)-4-methylcoumarin derivative in exts. of the trypanosome *Crithidia fasciculata*, was **purified** as the bimane derivative. Resonances attributable to U23 were discerned from those of the bimane label by comparison of the ¹H- and ¹³C-NMR spectra of monobromobimane and U23-bimane. The complete ¹H- and ¹³C-NMR spectra of U23-bimane were assigned by ¹H-¹H correlation spectroscopy, ¹H-¹³C correlation spectroscopy and ¹³C multiplicity detns. The results indicated identity of U23 with 1-N-methyl-4-mercaptohistidine (**ovothiol A**), previously isolated from marine sources. This assignment was confirmed by NOE difference expts., fast-atom-bombardment mass spectrometry of U23-bimane and UV/visible spectrophotometry of U23, which was isolated as the **disulfide**. The isolation of **ovothiol A** from a parasitic protozoan suggest that the 4-mercaptohistidines may have a wider distribution and function as antioxidant **thiols** than was hitherto realized.
- CC 10-1 (Microbial, Algal, and Fungal Biochemistry)
Section cross-reference(s): 6
- ST **ovothiol A** *Crithidia*
- IT *Crithidia fasciculata*
(**ovothiol A** of, identification and characterization of)
- IT 108418-13-9, **Ovothiol A**
RL: BIOL (Biological study)
(of *Crithidia fasciculata*, identification and characterization of)

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STRUCTURE FILE UPDATES: 27 SEP 2007 HIGHEST RN 948530-59-4

DICTIONARY FILE UPDATES: 27 SEP 2007 HIGHEST RN 948530-59-4

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FILE COVERS 1907 - 28 Sep 2007 VOL 147 ISS 15

FILE LAST UPDATED: 27 Sep 2007 (20070927/ED)

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'OBI' IS DEFAULT SEARCH FIELD FOR 'ZCAPLUS' FILE

=> d stat que L33

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| L14 | 264757 | SEA | FILE=ZCAPLUS | ABB=ON | PLU=ON | PUR/RL |
| L15 | 32 | SEA | FILE=ZCAPLUS | ABB=ON | PLU=ON | L13 (L) L14 |
| L16 | 118162 | SEA | FILE=ZCAPLUS | ABB=ON | PLU=ON | DISULFID?/BI |
| L17 | 147 | SEA | FILE=ZCAPLUS | ABB=ON | PLU=ON | DI SULFID?/BI |
| L18 | 1626 | SEA | FILE=ZCAPLUS | ABB=ON | PLU=ON | BISULFID?/BI OR BI SULFID?/BI |
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| L32 | 4 | SEA | FILE=ZCAPLUS | ABB=ON | PLU=ON | L19 AND 75-15-0?/OBI |
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=> d stat que L35

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| L5 | 1 | SEA | FILE=REGISTRY | ABB=ON | PLU=ON | 709044-44-0 |
| L6 | 1 | SEA | FILE=REGISTRY | ABB=ON | PLU=ON | 847493-45-2 |
| L8 | 1 | SEA | FILE=REGISTRY | ABB=ON | PLU=ON | 6088-50-2 |
| L9 | 1 | SEA | FILE=REGISTRY | ABB=ON | PLU=ON | 105988-28-1 |
| L10 | 1 | SEA | FILE=REGISTRY | ABB=ON | PLU=ON | 847493-44-1 |
| L11 | 1 | SEA | FILE=REGISTRY | ABB=ON | PLU=ON | 847493-46-3 |
| L24 | 120255 | SEA | FILE=ZCAPLUS | ABB=ON | PLU=ON | ?DISULFID?/BI |
| L25 | 167140 | SEA | FILE=ZCAPLUS | ABB=ON | PLU=ON | ?THIOL?/BI |
| L26 | 20268 | SEA | FILE=ZCAPLUS | ABB=ON | PLU=ON | L24 AND L25 |
| L31 | 14 | SEA | FILE=ZCAPLUS | ABB=ON | PLU=ON | (L3 OR L5 OR L6 OR (L8 OR L9 OR L10 OR L11)) AND L26 |
| L35 | 2 | SEA | FILE=ZCAPLUS | ABB=ON | PLU=ON | L31 AND ?ISOLAT?/OBI |

=> d stat que L36

| | | | | | | |
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| L8 | 1 | SEA | FILE=REGISTRY | ABB=ON | PLU=ON | 6088-50-2 |
| L9 | 1 | SEA | FILE=REGISTRY | ABB=ON | PLU=ON | 105988-28-1 |
| L10 | 1 | SEA | FILE=REGISTRY | ABB=ON | PLU=ON | 847493-44-1 |
| L11 | 1 | SEA | FILE=REGISTRY | ABB=ON | PLU=ON | 847493-46-3 |
| L24 | 120255 | SEA | FILE=ZCAPLUS | ABB=ON | PLU=ON | ?DISULFID?/BI |
| L25 | 167140 | SEA | FILE=ZCAPLUS | ABB=ON | PLU=ON | ?THIOL?/BI |
| L26 | 20268 | SEA | FILE=ZCAPLUS | ABB=ON | PLU=ON | L24 AND L25 |
| L31 | 14 | SEA | FILE=ZCAPLUS | ABB=ON | PLU=ON | (L3 OR L5 OR L6 OR (L8 OR L9 OR L10 OR L11)) AND L26 |
| L36 | 1 | SEA | FILE=ZCAPLUS | ABB=ON | PLU=ON | L31 AND TOTAL/TI |

=> d stat que L37

| | | | | | | |
|-----|--------|-----|---------------|--------|--------|--|
| L3 | 1 | SEA | FILE=REGISTRY | ABB=ON | PLU=ON | 192126-76-4 |
| L5 | 1 | SEA | FILE=REGISTRY | ABB=ON | PLU=ON | 709044-44-0 |
| L6 | 1 | SEA | FILE=REGISTRY | ABB=ON | PLU=ON | 847493-45-2 |
| L8 | 1 | SEA | FILE=REGISTRY | ABB=ON | PLU=ON | 6088-50-2 |
| L9 | 1 | SEA | FILE=REGISTRY | ABB=ON | PLU=ON | 105988-28-1 |
| L10 | 1 | SEA | FILE=REGISTRY | ABB=ON | PLU=ON | 847493-44-1 |
| L11 | 1 | SEA | FILE=REGISTRY | ABB=ON | PLU=ON | 847493-46-3 |
| L24 | 120255 | SEA | FILE=ZCAPLUS | ABB=ON | PLU=ON | ?DISULFID?/BI |
| L25 | 167140 | SEA | FILE=ZCAPLUS | ABB=ON | PLU=ON | ?THIOL?/BI |
| L26 | 20268 | SEA | FILE=ZCAPLUS | ABB=ON | PLU=ON | L24 AND L25 |
| L31 | 14 | SEA | FILE=ZCAPLUS | ABB=ON | PLU=ON | (L3 OR L5 OR L6 OR (L8 OR L9 OR L10 OR L11)) AND L26 |

L37 1 SEA FILE=ZCAPLUS ABB=ON PLU=ON L31 AND REDUCTION?/TI

=> d stat que L23

L14 264757 SEA FILE=ZCAPLUS ABB=ON PLU=ON PUR/RL
 L20 3625 SEA FILE=ZCAPLUS ABB=ON PLU=ON DISULFIDES/CT
 L21 7 SEA FILE=ZCAPLUS ABB=ON PLU=ON L20 (L) L14
 L22 167140 SEA FILE=ZCAPLUS ABB=ON PLU=ON ?THIOL?/BI
 L23 1 SEA FILE=ZCAPLUS ABB=ON PLU=ON L21 AND L22

=> d stat que L58

L14 264757 SEA FILE=ZCAPLUS ABB=ON PLU=ON PUR/RL
 L20 3625 SEA FILE=ZCAPLUS ABB=ON PLU=ON DISULFIDES/CT
 L21 7 SEA FILE=ZCAPLUS ABB=ON PLU=ON L20 (L) L14
 L39 166847 SEA FILE=ZCAPLUS ABB=ON PLU=ON ?MERCAPT?/BI
 L58 3 SEA FILE=ZCAPLUS ABB=ON PLU=ON L39 AND L21

=> d stat que L62

L5 1 SEA FILE=REGISTRY ABB=ON PLU=ON 709044-44-0
 L6 1 SEA FILE=REGISTRY ABB=ON PLU=ON 847493-45-2
 L11 1 SEA FILE=REGISTRY ABB=ON PLU=ON 847493-46-3
 L59 2 SEA FILE=ZCAPLUS ABB=ON PLU=ON L5
 L60 1 SEA FILE=ZCAPLUS ABB=ON PLU=ON L6
 L61 1 SEA FILE=ZCAPLUS ABB=ON PLU=ON L11
 L62 2 SEA FILE=ZCAPLUS ABB=ON PLU=ON (L59 OR L60 OR L61)

=> d stat que L69

L8 1 SEA FILE=REGISTRY ABB=ON PLU=ON 6088-50-2
 L10 1 SEA FILE=REGISTRY ABB=ON PLU=ON 847493-44-1
 L63 9 SEA FILE=ZCAPLUS ABB=ON PLU=ON L8
 L64 1 SEA FILE=ZCAPLUS ABB=ON PLU=ON L10
 L65 9 SEA FILE=ZCAPLUS ABB=ON PLU=ON (L63 OR L64)
 L68 15061 SEA FILE=ZCAPLUS ABB=ON PLU=ON MERCAPTO GROUP/CT
 L69 1 SEA FILE=ZCAPLUS ABB=ON PLU=ON L65 AND L68

=> d stat que L71

L3 1 SEA FILE=REGISTRY ABB=ON PLU=ON 192126-76-4
 L71 2 SEA FILE=ZCAPLUS ABB=ON PLU=ON L3/PUR

=> s (L33 or L35 or L36 or L37 or L23 or L58 or L62 or L69 or L71) not L55-L56
 L94 13 (L33 OR L35 OR L36 OR L37 OR L23 OR L58 OR L62 OR L69 OR L71)
 NOT (L55 OR L56)

=> file casreact

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FILE CONTENT:1840 - 22 Sep 2007 VOL 147 ISS 14

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*
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*
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=> d stat que L89

```
L86      1384 SEA FILE=CASREACT ABB=ON  PLU=ON  THIOL/FG.RCT (L) DISULFIDE/FG
        .PRO
L87      505 SEA FILE=CASREACT ABB=ON  PLU=ON  DISULFIDE/FG.RCT (L)
        THIOL/FG.PRO
L89      12 SEA FILE=CASREACT ABB=ON  PLU=ON  L86 (L) L87
```

=> dup rem L94 L89

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PROCESSING COMPLETED FOR L94
PROCESSING COMPLETED FOR L89
L95 25 DUP REM L94 L89 (0 DUPLICATES REMOVED)
 ANSWERS '1-13' FROM FILE ZCAPLUS
 ANSWERS '14-25' FROM FILE CASREACT

=> d ibib abs hitind hitstr L95 1-13; d ibib abs hit L95 14-25

```
L95  ANSWER 1 OF 25  ZCAPLUS  COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER:      2004:553613  ZCAPLUS  Full-text
DOCUMENT NUMBER:       141:239461
TITLE:                 Isolation and structure assignments of rostratins A-D,
                        cytotoxic disulfides produced by the marine-derived
                        fungus Exserohilum rostratum
AUTHOR(S):             Tan, Ren Xiang; Jensen, Paul R.; Williams, Philip G.;
                        Fenical, William
CORPORATE SOURCE:      Center for Marine Biotechnology and Biomedicine,
                        Scripps Institution of Oceanography, University of
                        California, La Jolla, CA, 92093-0204, USA
SOURCE:                Journal of Natural Products (2004), 67(8), 1374-1382
                        CODEN: JNPRDF; ISSN: 0163-3864
PUBLISHER:             American Chemical Society
DOCUMENT TYPE:         Journal
LANGUAGE:              English
GI
```

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Four new cytotoxic disulfides, rostratins A-D (I-IV), were isolated from the whole broth of the marine-derived fungus *E. rostratum* (Drechsler), a fungal strain found associated with a marine cyanobacterial mat. The structures of these cyclic dipeptides were established through chemical degradation and a variety of 2-dimensional NMR techniques. The absolute configurations of the rostratins were determined by the modified Mosher method. In the case of the polyhydroxylated compound I and the **mercaptol** IV, regioselective acylation was achieved by modulating the reaction temperature while monitoring the progress of the reaction by ¹H NMR. I, II, III, and IV showed in vitro cytotoxicity against human colon carcinoma (HCT-116) with IC₅₀ values of 8.5, 1.9, 0.76, and 16.5 µg/mL, resp.

CC 10-1 (Microbial, Algal, and Fungal Biochemistry)

IT **Disulfides**

RL: BSU (Biological study, unclassified); NPO (Natural product occurrence); PRP (Properties); **PUR (Purification or recovery)**;

BIOL (Biological study); OCCU (Occurrence); PREP (Preparation)

(rostratins A-D are cytotoxic disulfides produced by the marine-derived fungus *Exserohilum rostratum*)

REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L95 ANSWER 2 OF 25 ZCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2004:42415 ZCAPLUS Full-text

DOCUMENT NUMBER: 140:253784

TITLE: First **Total** Synthesis of **Mycothiols** and **Mycothiols Disulfide**

AUTHOR(S): Lee, Sungwon; Rosazza, John P. N.

CORPORATE SOURCE: Division of Medicinal and Natural Products Chemistry, College of Pharmacy, and Center for Biocatalysis and Bioprocessing, University of Iowa, Iowa City, IA, 52242, USA

SOURCE: Organic Letters (2004), 6(3), 365-368

CODEN: ORLEF7; ISSN: 1523-7060

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 140:253784

AB The first total synthesis of **mycothiol** and **mycothiol disulfide** was achieved by linking D-2,3,4,5,6-penta-O-acetyl-myo- inositol, O-(3,4,6-tri-O-acetyl-2-azido-2-deoxy- α,β -D- glucopyranosyl)trichloroacetimidate, and N,S-diacetyl-L-cysteine and deprotecting peracetylated **mycothiol**. The first full spectral characterization is reported for underivatized **mycothiol**. The structure of **mycothiol** was confirmed by spectral anal. of the known biman derivative

CC 33-7 (Carbohydrates)

Section cross-reference(s): 34

ST inositol azidodeoxyglucopyranose acetylcysteine conjugation **mycothiol** synthesis; **mycothiol** sulfide biman total synthesis

IT Cyclitols

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(first total synthesis of **mycothiol** and **mycothiol disulfide**)

IT Molecular structure

(of **mycothiol**)

IT **192126-76-4P**

RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP

(Preparation); RACT (Reactant or reagent)
 (first total synthesis of **mycothiol** and **mycothiol**
disulfide)

IT 52-89-1, L-Cysteine hydrochloride 87-89-8, myo-Inositol 1122-84-5,
 1-Ethoxycyclohexene 2873-29-2, Tri-O-acetyl-D-glucal 39637-74-6,
 (-)-Camphoric chloride 71418-44-5, Monobromobimane 145626-87-5,
 Bis(2-mercaptoethyl)sulfone

RL: RCT (Reactant); RACT (Reactant or reagent)
 (first total synthesis of **mycothiol** and **mycothiol**
disulfide)

IT 18725-37-6P 35519-39-2P 38183-33-4P 104873-71-4P 111901-82-7P
 111901-83-8P 120202-94-0P 145840-43-3P 187726-63-2P 668481-13-8P
 668481-14-9P 668481-15-0P 668481-16-1P 669091-43-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)

(first total synthesis of **mycothiol** and **mycothiol**
disulfide)

IT 158761-05-8P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (first total synthesis of **mycothiol** and **mycothiol**
disulfide)

IT 192126-76-4P

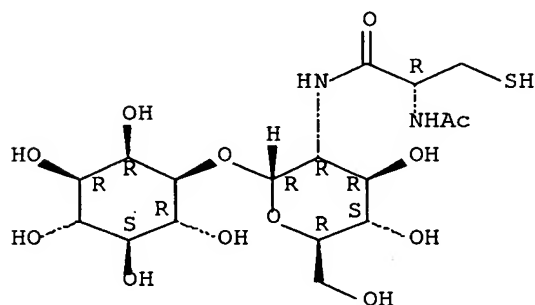
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP
 (Preparation); RACT (Reactant or reagent)

(first total synthesis of **mycothiol** and **mycothiol**
disulfide)

RN 192126-76-4 ZCAPLUS

CN D-myo-Inositol, 1-O-[2-[[[(2R)-2-(acetylamino)-3-mercapto-1-
 oxopropyl]amino]-2-deoxy- α -D-glucopyranosyl]- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L95 ANSWER 3 OF 25 ZCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2002:706948 ZCAPLUS Full-text

DOCUMENT NUMBER: 137:372244

TITLE: Mercaptans from Gas Condensates and Crude Oils

AUTHOR(S): Sharipov, A. Kh.

CORPORATE SOURCE: Institute of Petrochemistry and Catalysis, Academy of
 Sciences of the Republic of Bashkortostan and Urals
 Science Center, Russia

SOURCE: Chemistry and Technology of Fuels and Oils
 (Translation of Khimiya i Tekhnologiya Topliv i Masel)

(2002), 38(4), 280-285

CODEN: CTFOAK; ISSN: 0009-3092

PUBLISHER: Kluwer Academic/Consultants Bureau

DOCUMENT TYPE: Journal; General Review

LANGUAGE: English

AB A review on the occurrence of mercaptans in natural gas and petroleum and technologies for removal. Industrial separation schemes are described, and promising areas of application of mercaptans from gas condensate and kerosene distillates of medium-sulfur crude oils are noted. The fields of mercaptan-containing gas condensates and crude oils in regions confined to the Caspian Sea basin opened up with the development of deep drilling technol. For example, the Markovo field in East siberia has a high mercaptan content, 0.5-0.7%, the majority of the sulfur present, and has an absence of elemental sulfur, sulfide, and **disulfide** species. The Caspian Sea fields are also high in mercaptan sulfur and low in inorg. forms. Production of heavy carbonaceous crudes containing up to 50-80 ppm Me- and ethylmercaptans is increasing at high rates in the region between the Volga and the Urals, with even higher Et mercaptan concentration in the gas condensates. The mercaptans are extracted with alkali forming sodium salts, sent to another tower where they are thermally decomposed back into alkali and mercaptans. Currently in Russia, much of the mercaptans are wasted. Various strategies for com. products made from these mercaptans are presented. For example, methylmercaptan can be used to produce synthetic methionine by reacting with acrolein to form an aldehyde intermediate, reducing toxicity and odor of outgoing product shipments, but currently in Russia this material is mostly burned at the natural gas processing plants. Another example describes catalytic conversion to alkyl **disulfides**.

CC 51-0 (Fossil Fuels, Derivatives, and Related Products)

IT **Disulfides**RL: IMF (Industrial manufacture); PREP (Preparation)
(alkyl derivs.; recovery and uses of mercaptans from gas condensates and crude oils)IT **Thiols, preparation**RL: GOC (Geological or astronomical occurrence); **PUR (Purification or recovery)**; REM (Removal or disposal); OCCU (Occurrence); PREP
(Preparation); PROC (Process)

(recovery and uses of mercaptans from gas condensates and crude oils)

REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L95 ANSWER 4 OF 25 ZCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2001:770996 ZCAPLUS Full-text

DOCUMENT NUMBER: 135:305979

TITLE: Process for removing sulfur compounds from hydrocarbon streams

INVENTOR(S): Pittman, Rusty; Arena, Blaise J.; Janssen, Albert J.

PATENT ASSIGNEE(S): UOP LLC, USA

SOURCE: U.S., 6 pp., Cont.-in-part of U.S. Ser. No. 61,661, abandoned.

CODEN: USXXAM

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---------------|------|----------|-----------------|----------|
| US 6306288 | B1 | 20011023 | US 1999-426818 | 19991022 |
| EG 22909 | A | 20031030 | EG 2001-669 | 20010620 |
| JP 2003226881 | A | 20030815 | JP 2001-189890 | 20010622 |

| | | | | |
|---------------|----|----------|----------------|----------|
| JP 2003027068 | A | 20030129 | JP 2001-191421 | 20010625 |
| EP 1270704 | A1 | 20030102 | EP 2001-115343 | 20010626 |
| EP 1270704 | B1 | 20060927 | | |

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
IE, SI, LT, LV, FI, RO, MK, CY, AL, TR

| | | | | |
|-----------|---|----------|----------------|----------|
| AT 340837 | T | 20061015 | AT 2001-115343 | 20010626 |
|-----------|---|----------|----------------|----------|

PRIORITY APPLN. INFO.:

US 1998-61661 B2 19980417

US 1999-426818 A 19991022

EP 2001-115343 A 20010626

AB A process for removing H₂S and **mercaptans** from a hydrocarbon stream is disclosed. A hydrocarbon stream such as a LPG stream is contacted with a weakly basic stream, e.g., a Na bicarbonate stream to extract the H₂S and **mercaptans** from the hydrocarbon stream into the basic stream. The basic stream is now treated in a reactor containing a sulfide-oxidizing microorganism to convert the H₂S to S and the **mercaptans** to disulfides. Finally, the S and disulfides are separated from the basic aqueous stream which can be recycled and used to treat a fresh hydrocarbon stream. The treated hydrocarbon stream is purified to the point that it passes the Cu strip test, while the purified basic stream contains <0.08 g S/L.

IC ICM C10G019-08

ICS C10G019-00; C10G032-00

INCL 208235000

CC 51-4 (Fossil Fuels, Derivatives, and Related Products)

Section cross-reference(s): 49

ST sulfur compd removal hydrocarbon; hydrogen sulfide removal LPG;
mercaptan removal LPG

IT **Disulfides**RL: **PUR (Purification or recovery)**; PREP (Preparation)

(recovery in removing of sulfur compds. from hydrocarbon streams)

IT **Thiols** (organic), processes

RL: REM (Removal or disposal); PROC (Process)

(removing of sulfur compds. from hydrocarbon streams)

REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L95 ANSWER 5 OF 25 ZCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2001:381217 ZCAPLUS Full-text

DOCUMENT NUMBER: 135:166575

TITLE: Unexpected Catalyzed C:C Bond Cleavage by Molecular
Oxygen Promoted by a Thiyl Radical

AUTHOR(S): Baucherel, Xavier; Uziel, Jacques; Juge, Sylvain

CORPORATE SOURCE: Unite Mixte Universite de Cergy Pontoise-ESCOM FRE

CNRS 2126 Synthese Organique Selective et Chimie

Organometallique, Cergy Pontoise, 95031, Fr.

SOURCE: Journal of Organic Chemistry (2001), 66(13), 4504-4510

CODEN: JOCEAH; ISSN: 0022-3263

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 135:166575

AB Olefin oxidation with mol. oxygen, promoted by a transition metal catalyst and a thiophenol, involved C:C bond cleavage into the corresponding carbonyl derivs. This new reaction proceeds under one atmospheric of oxygen, at room temperature, in the presence of an excess of thiophenol and a catalyst such as MnL₂ 3a or VClL₂ 3c. It was applied to aromatic and aliphatic olefins, as well as to functionalized or unfunctionalized acyclic compds., providing the corresponding ketones and aldehydes in up to 98% yield. The synthetic interest of this catalytic oxidation was illustrated by a one-step preparation of the fragrance (-)-4-acetyl-1-methylcyclohexene 7e in 73% isolated yield. The C:C bond cleavage probably results from a catalyzed decomposition of the

β -hydroperoxysulfide intermediate that is formed by the radical addition of thiophenol to the olefin in the presence of oxygen. Although an excess of the thiophenol was used, it was transformed into the **disulfide** which could then be reduced without purification in 83% overall yield, thereby allowing for recycling. In addition, the C:C bond cleavage under oxygen could be promoted by catalytic quantities of the thiyl radical, generated by photolysis of the **disulfide**; thus, in the presence of 0.1 equiv of bis(4-chlorophenyl) **disulfide** 4b and 5% of the manganese complex 3a, trans-methylstilbene gave, under radiation, benzaldehyde and acetophenone in up to 95% yield. This new reaction offers an alternative to the classical C:C bond cleavage procedures, and further developments in the fields of bioinorg. and environmental chemical are likely.

CC 22-7 (Physical Organic Chemistry)

Section cross-reference(s): 30, 62

IT Aromatic hydrocarbons, reactions

RL: PEP (Physical, engineering or chemical process); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)

(aryl alkenes; oxidative bond cleavage of olefins with mol. oxygen promoted by transition metal complex catalyst and a thiophenol and its photochem. version with transition metal complex and catalytic **disulfide**)

IT **Thiols (organic), reactions**

RL: CAT (Catalyst use); PEP (Physical, engineering or chemical process);

PUR (Purification or recovery); RCT (Reactant); PREP

(Preparation); PROC (Process); RACT (Reactant or reagent); USES (Uses)

(aryl; oxidative bond cleavage of olefins with mol. oxygen promoted by transition metal complex catalyst and a thiophenol and its photochem. version with transition metal complex and catalytic **disulfide**)

)

IT Alkenes, reactions

RL: PEP (Physical, engineering or chemical process); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)

(aryl; oxidative bond cleavage of olefins with mol. oxygen promoted by transition metal complex catalyst and a thiophenol and its photochem. version with transition metal complex and catalytic **disulfide**)

)

IT **Disulfides**

RL: CAT (Catalyst use); FMU (Formation, unclassified); RCT (Reactant);

FORM (Formation, nonpreparative); RACT (Reactant or reagent); USES (Uses)

(formation and reduction under thermal conditions and catalytic activity under photolytic conditions)

IT Catalysts

Regiochemistry

(oxidative bond cleavage of olefins with mol. oxygen promoted by transition metal complex catalyst and a thiophenol and its photochem. version with transition metal complex and catalytic **disulfide**)

)

IT Transition metal complexes

RL: CAT (Catalyst use); USES (Uses)

(oxidative bond cleavage of olefins with mol. oxygen promoted by transition metal complex catalyst and a thiophenol and its photochem. version with transition metal complex and catalytic **disulfide**)

)

IT Alkenes, reactions

RL: PEP (Physical, engineering or chemical process); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)

(oxidative bond cleavage of olefins with mol. oxygen promoted by transition metal complex catalyst and a thiophenol and its photochem. version with transition metal complex and catalytic **disulfide**)

)

- IT Aldehydes, preparation
Ketones, preparation
RL: SPN (Synthetic preparation); PREP (Preparation)
(oxidative bond cleavage of olefins with mol. oxygen promoted by transition metal complex catalyst and a thiophenol and its photochem. version with transition metal complex and catalytic **disulfide**)
- IT Bond cleavage
(oxidative; oxidative bond cleavage of olefins with mol. oxygen promoted by transition metal complex catalyst and a thiophenol and its photochem. version with transition metal complex and catalytic **disulfide**)
- IT Photolysis
(photoinduced C:C bond cleavage; oxidative bond cleavage of olefins with mol. oxygen promoted by transition metal complex catalyst and a thiophenol and its photochem. version with transition metal complex and catalytic **disulfide**)
- IT Phenols, reactions
RL: CAT (Catalyst use); PEP (Physical, engineering or chemical process); PUR (Purification or recovery); RCT (Reactant); PREP (Preparation); PROC (Process); RACT (Reactant or reagent); USES (Uses)
(thiophenols; oxidative bond cleavage of olefins with mol. oxygen promoted by transition metal complex catalyst and a thiophenol and its photochem. version with transition metal complex and catalytic **disulfide**)
- IT 151930-49-3P
RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(catalytic ligand; oxidative bond cleavage of olefins with mol. oxygen promoted by transition metal complex catalyst and a thiophenol and its photochem. version with transition metal complex and catalytic **disulfide**)
- IT 90-02-8, Salicylaldehyde, reactions 5619-04-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(condensation; oxidative bond cleavage of olefins with mol. oxygen promoted by transition metal complex catalyst and a thiophenol and its photochem. version with transition metal complex and catalytic **disulfide**)
- IT 353736-48-8
RL: FMU (Formation, unclassified); FORM (Formation, nonpreparative)
(not a bond cleavage intermediate; oxidative bond cleavage of olefins with mol. oxygen promoted by transition metal complex catalyst and a thiophenol and its photochem. version with transition metal complex and catalytic **disulfide**)
- IT 1142-19-4, Bis(4-chlorophenyl) **disulfide** 7718-98-1, Vanadium trichloride 7773-01-5, Manganese dichloride
RL: CAT (Catalyst use); USES (Uses)
(oxidative bond cleavage of olefins with mol. oxygen promoted by transition metal complex catalyst and a thiophenol and its photochem. version with transition metal complex and catalytic **disulfide**)
- IT 100-42-5, Styrene, reactions 103-30-0, trans-Stilbene 111-66-0, 1-Octene 140-10-3, trans-Cinnamic acid, reactions 447-53-0, 1,2-Dihydronaphthalene 530-48-3, 1,1-Diphenylethylene 623-91-6, Ethyl fumarate 645-49-8, cis-Stilbene 695-12-5, Vinylcyclohexane 833-81-8, trans-1,2-Diphenylpropene 4192-77-2, trans-Ethyl cinnamate 4407-36-7, trans-Cinnamyl alcohol 5989-54-8, (S)-(-)-Limonene 6094-02-6, 2-Methyl-1-hexene 7782-44-7, Oxygen, reactions 18172-67-3, (-)- β -Pinene
RL: PEP (Physical, engineering or chemical process); RCT (Reactant); PROC

(Process); RACT (Reactant or reagent)
 (oxidative bond cleavage of olefins with mol. oxygen promoted by
 transition metal complex catalyst and a thiophenol and its photochem.
 version with transition metal complex and catalytic **disulfide**
)

IT 98-86-2P, Acetophenone, preparation 100-52-7P, Benzaldehyde, preparation
 111-71-7P, Heptanal 119-61-9P, Benzophenone, preparation 591-78-6P,
 2-Hexanone 924-44-7P, Ethyl glyoxylate 2043-61-0P,
 Cyclohexanecarboxaldehyde 14807-28-4P 38651-65-9P, (+)-Nopinone
 57072-59-0P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (oxidative bond cleavage of olefins with mol. oxygen promoted by
 transition metal complex catalyst and a thiophenol and its photochem.
 version with transition metal complex and catalytic **disulfide**
)

IT 106-54-7P, 4-Chlorothiophenol 7340-90-1P

RL: CAT (Catalyst use); PEP (Physical, engineering or chemical process);
 PUR (Purification or recovery); RCT (Reactant); PREP (Preparation); PROC
 (Process); RACT (Reactant or reagent); USES (Uses)
 (reagent and recovery; oxidative bond cleavage of olefins with mol.
 oxygen promoted by transition metal complex catalyst and a thiophenol
 and its photochem. version with transition metal complex and catalytic
disulfide)

REFERENCE COUNT: 55 THERE ARE 55 CITED REFERENCES AVAILABLE FOR THIS
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L95 ANSWER 6 OF 25 ZCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2000:439719 ZCAPLUS Full-text

DOCUMENT NUMBER: 133:204979

TITLE: Contamination of an anion-exchange membrane by
 glutathione

AUTHOR(S): Gotoh, Takeshi; Kikuchi, Ken-Ichi

CORPORATE SOURCE: Department of Materials-Process Engineering & Applied
 Chemistry for Environments, Faculty of Engineering and
 Resource Science, Akita University, Akita, 010-8502,
 Japan

SOURCE: Bioseparation (2000), 9(1), 37-41

CODEN: BISPE4; ISSN: 0923-179X

PUBLISHER: Kluwer Academic Publishers

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Electrodialysis, which can sep. electrolytes under mild conditions by using
 ion-exchange membranes, is a strong candidate for separation of GSH from yeast
 exts., because GSH is unstable and easily oxidized forming a **disulfide** bond
 especially under alkali conditions. In this paper, sorption behavior of GSH
 on an anion-exchange membrane, in the pH 3-6 region that is expected to be the
 most preferable for its electrodialytic separation, was examined Sorption of
 GSH on a Selemion-AMV anion-exchange membrane was accelerated as the pH of the
 membrane-contact solution increased, and there was a good correlation between
 the sorbed amts. and the molar fraction of monovalent anionic species of GSH.
 However, the amts. of GSH desorbed from the membrane by a NaCl desorbing
 solution were much lower than the initial sorbed amts., and the difference
 between them was enlarged with increasing pH. The GSH which was lost could be
 recovered by the addition of DTT in the membrane-contact and desorbing solns.
 Similar results were also obtained with Cys. We thus concluded that an anion-
 exchange membrane would be contaminated by thiol compds., such as GSH and Cys,
 through oxidative binding of the thiol group with the membrane, the local OH-
 concentration in which was enhanced due to attraction by the pos. charged
 anion-exchange membrane.

CC 9-9 (Biochemical Methods)

Section cross-reference(s): 6, 34

IT **Thiols (organic), biological studies**

RL: BPR (Biological process); BSU (Biological study, unclassified); PEP (Physical, engineering or chemical process); **PUR (Purification or recovery)**; BIOL (Biological study); PREP (Preparation); PROC (Process)

(contamination of anion-exchange membrane by glutathione)

REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L95 ANSWER 7 OF 25 ZCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1999:341203 ZCAPLUS Full-text

DOCUMENT NUMBER: 130:339677

TITLE: Process for preparing pure and stable solutions of organic thiols, sulfides and dithiocarbamates

INVENTOR(S): Svehla, Pavel; Zaludek, Borek; Rosicky, Lubor

PATENT ASSIGNEE(S): Lachema, A. S., Czech Rep.

SOURCE: Czech Rep., 4 pp.

CODEN: CZXXED

DOCUMENT TYPE: Patent

LANGUAGE: Czech

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------------------------|------|----------|-----------------|------------|
| CZ 283636 | B6 | 19980513 | CZ 1990-3560 | 19900718 |
| PRIORITY APPLN. INFO.: | | | CS 1990-3560 | A 19900718 |

AB Pure stable solns. of organic thiols, sulfides and dithiocarbaminates (e.g. sodium dimethyldithiocarbamate) are prepared from the corresponding crude organic compds. treatment with compds. (e.g., tetramethylthiuram **disulfide** and hydrazine sulfate) producing solid **disulfides** from the impurities at pH 10-12 followed by filtration of the solid **disulfide** impurity.

IC ICM C07C323-00

CC 45-1 (Industrial Organic Chemicals, Leather, Fats, and Waxes)

IT **Disulfides**

RL: BYP (Byproduct); REM (Removal or disposal); PREP (Preparation); PROC (Process)

(organic; removal of)

IT Thioethers

Thiols (organic), preparation

RL: **PUR (Purification or recovery)**; PREP (Preparation)

(process for preparing pure and stable solns. of)

IT Filtration

(process for preparing pure and stable solns. of organic thiols and sulfides

and dithiocarbamates with solid **disulfide** removal by)

IT 87-90-1, Trichloroisocyanuric acid 137-26-8, Tetramethylthiuram **disulfide** 302-01-2, Hydrazine, reactions 7722-64-7, Potassium permanganate 7722-84-1, Hydrogen peroxide, reactions 7727-21-1, Potassium peroxydisulfate 7775-14-6, Sodium dithionite 7803-49-8, Hydroxylamine, reactions 10034-93-2, Hydrazine sulfate

RL: RCT (Reactant); RACT (Reactant or reagent)

(process for preparing pure and stable solns. of organic thiols, sulfides

and dithiocarbamates)

L95 ANSWER 8 OF 25 ZCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1997:641496 ZCAPLUS Full-text

DOCUMENT NUMBER: 127:328617

TITLE: General method to identify and enrich vicinal thiol proteins present in intact cells in the oxidized, **disulfide** state

AUTHOR(S): Gitler, Carlos; Zarmi, Batia; Kalef, Edna

CORPORATE SOURCE: Dep. Membrane Res. Biophysics, Weizmann Inst. Sci., Rehovot, 76100, Israel

SOURCE: Analytical Biochemistry (1997), 252(1), 48-55
CODEN: ANBCA2; ISSN: 0003-2697

PUBLISHER: Academic

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Some 5% of the soluble proteins of L1210 murine leukemia lymphoblasts contain surface vicinal thiols. Redox dithiol to intraprotein **disulfide** conversion could regulate the cellular function of these proteins. A general method is presented to identify and enrich vicinal thiol proteins existing in cells in their oxidized, **disulfide** state. The method is based on the in situ blockage by cell permeable N-ethylmaleimide (NEM) of readily accessible cellular protein sulfhydryls. Following removal of the excess NEM, **disulfide**-containing proteins were identified by reduction with DTT and specific labeling with N-iodoacetyl-[125I]-3-iodotyrosine ([125I]IAIT). The vicinal thiol proteins formed could also be enriched, prior to labeling with [125I]IAIT, by their selective binding to Sepharose-aminohexanoyl-4-aminophenylarsine oxide. Exponentially growing L1210 lymphoblasts contain >20 proteins with thiols in the oxidized, **disulfide** state. The majority derive from vicinal thiol proteins. The fraction oxidized, in some proteins, represents almost the totality of the protein present in the cell. Exposure of lymphoblasts to diamide increases the number and concentration of proteins with intraprotein **disulfides**. This method allows sensitive direct identification of vicinal thiol proteins that participate in redox regulation and those that are targets to oxidative stress conditions.

CC 9-16 (Biochemical Methods)
Section cross-reference(s): 4

IT Animal cell line
(L-1210; identification and enrichment of vicinal thiol proteins present in cells in oxidized **disulfide** state)

IT Proteins, specific or class
RL: ANT (Analyte); PUR (Purification or recovery); ANST (Analytical study); PREP (Preparation)
(**disulfide**-containing; identification and enrichment of vicinal thiol proteins present in cells in oxidized **disulfide** state)

IT Thiols (organic), biological studies
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(dithiols; identification and enrichment of vicinal thiol proteins present in cells in oxidized **disulfide** state)

IT Lymphoblast
Oxidative stress, biological
(identification and enrichment of vicinal thiol proteins present in cells in oxidized **disulfide** state)

IT **Disulfides**
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(identification and enrichment of vicinal thiol proteins present in cells in oxidized **disulfide** state)

IT Proteins, specific or class
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(redox; identification and enrichment of vicinal thiol proteins present in cells in oxidized **disulfide** state)

IT Proteins, specific or class
RL: ANT (Analyte); PUR (Purification or recovery); ANST (Analytical

study); PREP (Preparation)

(vicinal thiol-containing; identification and enrichment of vicinal thiol proteins present in cells in oxidized **disulfide** state)

IT **Thiols (organic), analysis**

RL: ANT (Analyte); **PUR (Purification or recovery)**; ANST

(Analytical study); PREP (Preparation)

(vicinal, proteins containing; identification and enrichment of vicinal thiol proteins present in cells in oxidized **disulfide** state)

IT 128-53-0 150956-52-8

RL: ARG (Analytical reagent use); ANST (Analytical study); USES (Uses)
(identification and enrichment of vicinal thiol proteins present in cells in oxidized **disulfide** state)

IT 1122-90-3D, 4-Aminophenylarsine oxide, linked to aminohexanoyl and Sepharose 4B 1319-82-0D, Aminohexanoic acid, linked to Sepharose 4B and 4-aminophenylarsine oxide 9012-36-6D, Sepharose 4B, linked to aminohexanoyl and 4-aminophenylarsine oxide

RL: ARU (Analytical role, unclassified); ANST (Analytical study)
(identification and enrichment of vicinal thiol proteins present in cells in oxidized **disulfide** state)

IT 3483-12-3, Dithiothreitol

RL: RCT (Reactant); RACT (Reactant or reagent)

(identification and enrichment of vicinal thiol proteins present in cells in oxidized **disulfide** state)

REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L95 ANSWER 9 OF 25 ZCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1996:58340 ZCAPLUS Full-text

DOCUMENT NUMBER: 124:121805

TITLE: Separately removing **mercaptans** and hydrogen sulfide from gas streams with disulfide recovery

INVENTOR(S): Samuels, Alvin; Fox, Irwin

PATENT ASSIGNEE(S): USA

SOURCE: U.S., 5 pp. Cont.-in-part of U.S. 187,146, abandoned.
CODEN: USXXAM

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------------------------|------|----------|-----------------|-------------|
| US 5478541 | A | 19951226 | US 1995-440114 | 19950512 |
| PRIORITY APPLN. INFO.: | | | US 1995-440114 | B2 19950512 |
| | | | US 1994-187146 | 19940127 |

AB **Mercaptans** and hydrogen sulfide are removed sep. from a hydrocarbon gas stream by passing the gas through a bed which includes iron oxide (crystalline Fe₃O₄ and amorphous Fe₂O₃) which catalyzes the formation of disulfides and trisulfides from **mercaptans** and also reacts with at least part of the hydrogen sulfide to form acid-stable solids; causing the di- and trisulfides to exit the bed in the gas phase; and removing and recovering the di- and trisulfides by adsorption or condensation. Any remaining hydrogen sulfide may be scavenged from the gas stream by passage through a bed containing iron oxide similar to that used first above. If the gas stream contains substantial amts. of hydrocarbon aerosols, they should be filtered out in advance of the bed.

IC ICM C01B017-16

ICS C01B017-20

INCL 423220000

CC 51-5 (Fossil Fuels, Derivatives, and Related Products)

- ST **mercaptan** removal hydrocarbon gas disulfide recovery
- IT **Disulfides**
Trisulfides
RL: **PUR (Purification or recovery)**; REM (Removal or disposal);
PREP (Preparation); PROC (Process)
(sep. removing **mercaptans** and hydrogen sulfide from gas
streams with disulfide recovery)
- IT 7440-44-0, Carbon, uses
RL: NUU (Other use, unclassified); USES (Uses)
(activated; sep. removing **mercaptans** and hydrogen sulfide
from gas streams with disulfide recovery)
- IT 1309-37-1, Iron oxide (fe2o3), uses
RL: NUU (Other use, unclassified); USES (Uses)
(amorphous; sep. removing **mercaptans** and hydrogen sulfide
from gas streams with disulfide recovery)
- IT 1317-61-9, Iron oxide (fe3o4), uses
RL: NUU (Other use, unclassified); USES (Uses)
(crystalline; sep. removing **mercaptans** and hydrogen sulfide from
gas streams with disulfide recovery)
- IT 110-81-6P, Di ethyl disulfide 624-92-0P, Di methyl disulfide
3600-24-6P, Di ethyl trisulfide 3658-80-8P, Di methyl trisulfide
20333-39-5P, Methyl ethyl disulfide 31499-71-5P, Methyl ethyl trisulfide
RL: **PUR (Purification or recovery)**; REM (Removal or disposal); PREP
(Preparation); PROC (Process)
(sep. removing **mercaptans** and hydrogen sulfide from gas
streams with disulfide recovery)
- IT 74-93-1, Methyl **mercaptan**, processes 75-08-1, Ethyl
mercaptan 7783-06-4, Hydrogen sulfide, processes
RL: REM (Removal or disposal); PROC (Process)
(sep. removing **mercaptans** and hydrogen sulfide from gas
streams with disulfide recovery)

L95 ANSWER 10 OF 25 ZCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1995:630956 ZCAPLUS Full-text

DOCUMENT NUMBER: 124:140470

TITLE: The structure of U17 isolated from Streptomyces
clavuligerus and its properties as an antioxidant
thiol

AUTHOR(S): Newton, Gerald L.; Bewley, Carole A.; Dwyer, Tammy J.;
Horn, Ronda; Aharonowitz, Yair; Cohen, Gerald; Davies,
Julian; Faulkner, D. John; Fahey, Robert C.

CORPORATE SOURCE: Department of Chemistry and Biochemistry, University
of California, San Diego, La Jolla, CA, 92093-0506,
USA

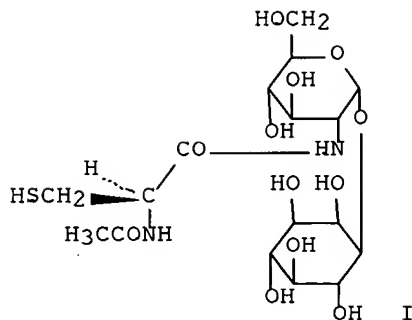
SOURCE: European Journal of Biochemistry (1995), 230(2), 821-5
CODEN: EJBCAI; ISSN: 0014-2956

PUBLISHER: Springer

DOCUMENT TYPE: Journal

LANGUAGE: English

GI



AB The predominant low-mol.-mass thiol produced by streptomycetes is a cysteine derivative previously designated as U17. In this study the elucidation of the structure of the monobromobimane derivative of U17 (I) is reported, which establishes the structure of U17 as 2-(N-acetylcysteinyl)amido-2-deoxy- α -D-glucopyranosyl-myo-inositol. The presence of the N-acetylcysteine moiety was indicated by formation of N-acetylcysteine-monobromobimane during acid hydrolysis of I. Complete hydrolysis of I released 1 mol glucosamine/mol cysteine as determined by carbohydrate and amino acid anal. High-resolution mass spectral anal. gave a precise mass consistent with the mol. formula C₂₇H₄₀N₄O₁₄S. Anal. of ¹³C-NMR, 1-dimensional ¹H-NMR and 2-dimensional NMR expts. identified the remaining C₆H₁₂O₆ moiety as myo-inositol, confirmed the presence of N-acetyl-cysteine and glucosamine, and established the connectivity of the components. Two chemical properties of this novel thiol, which is equated to mycothiol from Mycobacterium bovis, make it suitable as an intracellular storage form of cysteine and as an antioxidant thiol. First, it undergoes heavy-metal-ion catalyzed autoxidn. at a rate dramatically lower than that for cysteine and markedly lower than that for glutathione or N-acetylcysteine. Secondly, the α -(1 \rightarrow 1) glycosidic link between glucosamine and myo-inositol is resistant to acid hydrolysis, hydrolyzing at a rate comparable to that of the 2 amide bonds in the mol.

CC 10-1 (Microbial, Algal, and Fungal Biochemistry)

IT 158761-05-8P **192126-76-4P**, Mycothiol

RL: BAC (Biological activity or effector, except adverse); BPR (Biological process); BSU (Biological study, unclassified); PRP (Properties); **PUR (Purification or recovery)**; BIOL (Biological study); PREP (Preparation); PROC (Process)

(structure of U17 (mycothiol) isolated from Streptomyces clavuligerus and its properties as an antioxidant thiol)

IT **192126-76-4P**, Mycothiol

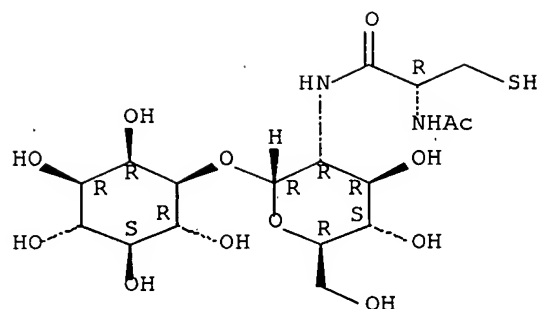
RL: BAC (Biological activity or effector, except adverse); BPR (Biological process); BSU (Biological study, unclassified); PRP (Properties); **PUR (Purification or recovery)**; BIOL (Biological study); PREP (Preparation); PROC (Process)

(structure of U17 (mycothiol) isolated from Streptomyces clavuligerus and its properties as an antioxidant thiol)

RN 192126-76-4 ZCAPLUS

CN D-myo-Inositol, 1-O-[2-[[(2R)-2-(acetylamino)-3-mercapto-1-oxopropyl]amino]-2-deoxy- α -D-glucopyranosyl]- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



L95 ANSWER 11 OF 25 ZCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1988:34449 ZCAPLUS Full-text

DOCUMENT NUMBER: 108:34449

TITLE: Purification of thiols from biological samples

AUTHOR(S): Newton, Gerald L.; Fahey, Robert C.

CORPORATE SOURCE: Dep. Chem., Univ. California, San Diego, La Jolla, CA, 92093, USA

SOURCE: Methods in Enzymology (1987), 143(Sulfur Sulfur Amino Acids), 96-101

CODEN: MENZAU; ISSN: 0076-6879

DOCUMENT TYPE: Journal; General Review

LANGUAGE: English

AB A 2-step purification procedure is described that allows a low-mol.-weight thiol component in a biol. extract to be isolated as the monobromobimane derivative in highly purified form. The thiols present in a deproteinized extract were first isolated on a thiol-agarose gel by a thiol-**disulfide** exchange reaction. The thiols were then eluted with dithiothreitol and derivatized with monobromobimane. The derivative was purified to homogeneity by preparative HPLC. A procedure for electrolytic reduction of the bimane derivative was developed that allows regeneration of the thiol form of the purified product. Application of the method is illustrated for isolation of a major thiol component found in Halobacterium halobium, the structure of which was shown to correspond to γ -glutamylcysteine.

CC 9-15 (Biochemical Methods)

IT **Thiols, preparation**

RL: **PUR (Purification or recovery)**; PREP (Preparation)
(purification of, from biol. samples)

L95 ANSWER 12 OF 25 ZCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1966:77583 ZCAPLUS Full-text

DOCUMENT NUMBER: 64:77583

ORIGINAL REFERENCE NO.: 64:14585g-h

TITLE: Specificity of the dihydroxydinaphthyl disulfide (DDD) reaction

AUTHOR(S): Gabler, W.; Scheuner, G.

CORPORATE SOURCE: Karl Marx Univ., Leipzig, Germany

SOURCE: Acta Histochem. (1966), 23(1-4), 102-9

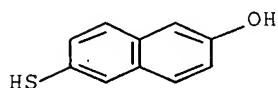
DOCUMENT TYPE: Journal

LANGUAGE: German

AB The DDD reaction between protein-bound SH groups and the reagent 2,2'-dihydroxy-6,6'-dinaphthyl disulfide was said to be specific, except for some interference by 6-mercapto-2-naphthol produced during the reaction. High concns. of SH groups gave a blue, low concns, a red color reaction with Fast Blue B salt. Pretreatment of tissue slices with chloramine T greatly

intensified the color of the DDD reaction when different oxidizing agents were compared. Esterification of primary carboxyl groups produced an intense blue-violet color which might be mistaken for a high concentration of SH or SS groups. The reaction is not understood. 21 references.

CC 60 (Biochemical Methods)
 IT **Mercapto group**
 (in proteins, reaction with 2,2'-dihydroxy-6,6'-dinaphthyl disulfide)
 IT **6088-50-2**, 2-Naphthol, 6-mercapto-
 (in protein bound mercapto group reaction with 2,2'-dihydroxy-6,6'-dinaphthyl disulfide)
 IT **6088-50-2**, 2-Naphthol, 6-mercapto-
 (in protein bound mercapto group reaction with 2,2'-dihydroxy-6,6'-dinaphthyl disulfide)
 RN 6088-50-2 ZCAPLUS
 CN 2-Naphthalenol, 6-mercapto- (9CI) (CA INDEX NAME)

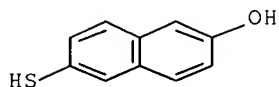


L95 ANSWER 13 OF 25 ZCAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 1958:50882 ZCAPLUS
 DOCUMENT NUMBER: 52:50882
 ORIGINAL REFERENCE NO.: 52:9214g-h
 TITLE: **Reduction of organic disulfides**
 INVENTOR(S): Gutcho, Marcia; Laufer, Louis
 PATENT ASSIGNEE(S): United States of America, as represented by the Secy.
 of the Navy
 DOCUMENT TYPE: Patent
 LANGUAGE: Unavailable
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------------|------|----------|-----------------|----------|
| US 2820780 | | 19580121 | US 1953-389479 | 19531030 |

AB Acid-insol. metallic sulfides of mol. weight over 60 (especially those of Bi, Pb, and Hg) catalyze the reaction of H₂S with organic **disulfides**, RSSR' (R and R' may be amino acid, peptide, alkyl, or aryl groups), to produce their **thiols**, RSH and R'SH. The reduction proceeds at room temperature and atmospheric pressure and the sulfide may be pre-formed or formed in situ. To 6% aqueous solution of oxidized glutathione (GSSG) 10 is added 10% aqueous solution Pb(OAc)₂·3H₂O 1 part and H₂S is bubbled into the solution. After the PbS is removed by filtration, GSH may be recovered as its Cu salt. Using H₂S, cystine is reduced to cysteine in 75% yield. Similarly, with Bi₂S₃, 2,2'-dihydroxy-6,6'-dinaphthyl **disulfide** yields 70% 2,6-thionaphthol.

CC 10 (Organic Chemistry)
 IT **6088-50-2P**, 2-Naphthol, 6-mercapto-
 RL: PREP (Preparation)
 (preparation of)
 IT **6088-50-2P**, 2-Naphthol, 6-mercapto-
 RL: PREP (Preparation)
 (preparation of)
 RN 6088-50-2 ZCAPLUS
 CN 2-Naphthalenol, 6-mercapto- (9CI) (CA INDEX NAME)



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L95 ANSWER 14 OF 25 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 145:460148 CASREACT Full-text

TITLE: Synthesis of Poly(β -amino ester)s with
Thiol-Reactive Side Chains for DNA Delivery

AUTHOR(S): Zugates, Gregory T.; Anderson, Daniel G.; Little,
Steven R.; Lawhorn, Ingrid E. B.; Langer, Robert

CORPORATE SOURCE: Department of Chemical Engineering, Massachusetts
Institute of Technology, Cambridge, MA, 02139, USA

SOURCE: Journal of the American Chemical Society (2006),
128(39), 12726-12734

CODEN: JACSAT; ISSN: 0002-7863

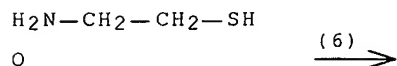
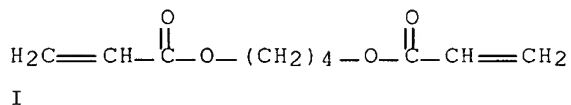
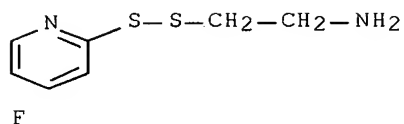
PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

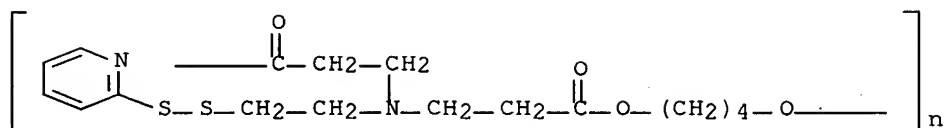
LANGUAGE: English

AB The safe and efficient delivery of DNA remains the major barrier to the clin. application of non-viral gene therapy. Here, we present novel, biodegradable polymers for gene delivery that are capable of simple graft modification and demonstrate the ability to respond to intracellular conditions. We synthesized poly(β -amino ester)s using a new amine monomer, 2-(pyridyldithio)-ethylamine (PDA). These cationic, degradable polymers contain pyridyldithio functionalities in the side chains that react with high specificity toward thiol ligands. This reactivity is demonstrated using both mercaptoethylamine (MEA) and the thiol peptide RGDC, a ligand that binds with high affinity to certain integrin receptors. These two polymer derivs. displayed strong DNA binding as determined using electrophoresis and dye exclusion assays. In addition, the MEA-based polymer and plasmid DNA were shown to self-assemble into cationic complexes with effective diams. as low as 100 nm. Furthermore, this DNA binding ability was substantially reduced in response to intracellular glutathione concns., which may aid in DNA unpackaging inside the cell. These complexes also displayed low cellular toxicity and were able to mediate transfection at levels comparable to PEI in human hepatocellular carcinoma cells. These results suggest that PDA-based poly(β -amino ester)s may serve as a modular platform for polymer-mediated gene delivery.

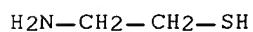
RX(6) OF 18 ... **F** + I + O ==> **P** +
Q



(6) →



P
 reaction produ
 ct with mercap
 toethylamine **O**



O
 reaction produ
 ct with 2-(Pyr
 idyldithio)-et

RX(6) RCT **F 83578-21-6**, **I 1070-70-8**

STAGE(1)

CON 2 days, 60 deg C

STAGE(2)

RCT **O 60-23-1**

SOL 67-68-5 DMSO

CON room temperature

PRO **P 913399-31-2D**, **Q 60-23-1D**

NTE no solvent (first stage)

REFERENCE COUNT:

49

THERE ARE 49 CITED REFERENCES AVAILABLE FOR THIS
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L95 ANSWER 15 OF 25 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 143:378542 CASREACT Full-textTITLE: Characterisation and biodistribution of two neutral $^{99m}\text{Tc}(\text{CO})_3$ complexes with a tridentate ligand

AUTHOR(S): Rattat, Dirk; Cleynhens, Bernard; Bormans, Guy; Terwinghe, Christelle; Verbruggen, Alfons

CORPORATE SOURCE: Laboratory for Radiopharmaceutical Chemistry and Nuclear Medicine, Catholic University of Leuven, Louvain, 3000, Belg.

SOURCE: Bioorganic & Medicinal Chemistry Letters (2005), 15(19), 4192-4195

CODEN: BMCLE8; ISSN: 0960-894X

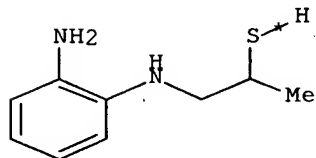
PUBLISHER: Elsevier B.V.

DOCUMENT TYPE: Journal

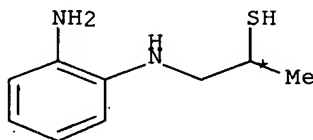
LANGUAGE: English

AB N-(2-Mercapto-propyl)-1,2-phenylenediamine (MPPDA) and N- β -aminoethylglycine (AEG) were labeled with $^{99m}\text{Tc}(\text{CO})_3^+$ to form the neutral complexes $[\text{MPPDA}]$ and $[\text{AEG}]$. Both complexes were formed in excellent yields and their identities were confirmed by LC-MS. In mice, none of the new tracer agents showed brain uptake. $[\text{MPPDA}]$ was trapped mainly in the liver and excreted via the hepatobiliary system, whereas $[\text{AEG}]$ was excreted rapidly via the kidneys to the urine.

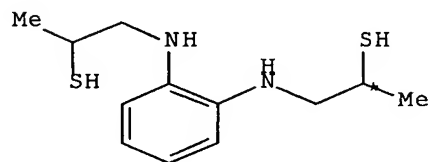
RX(2) OF 6 ... 2 C + 2 D + E + 2 F ==>
G + H + I



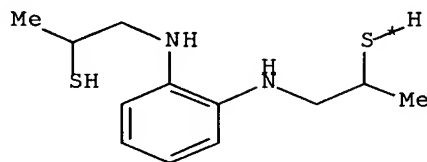
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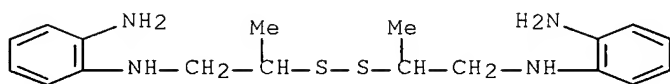
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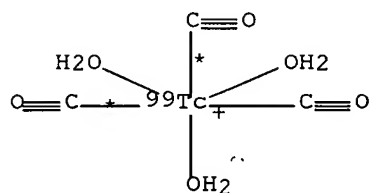
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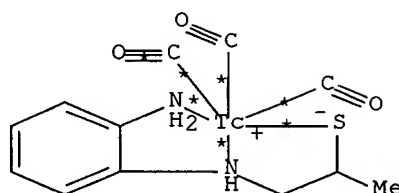
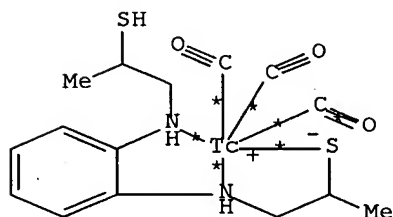
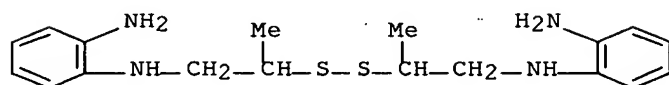


E



2 F

(2) →

G
YIELD 57%H
YIELD 27%I
YIELD 17%
reaction produ
ct with technet
ium-99m triaqua

RX(2) RCT C 245059-12-5, D 255379-03-4, E
866395-63-3, F 163932-31-8
PRO G 866395-64-4, H 866395-65-5, I 866395-63-3D
CON 30 minutes, 70 deg C, pH 10
NTE product with technetium-99m triaqua tricarbonyl
REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L95 ANSWER 16 OF 25 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 139:303501 CASREACT Full-text

TITLE: The role of cystine knots in collagen folding and stability, part I. Conformational properties of (Pro-Hyp-Gly)5 and (Pro-(4S)-FPro-Gly)5 model trimers with an artificial cystine knot

AUTHOR(S): Barth, Dirk; Musiol, Hans-Juergen; Schuett, Markus; Fiori, Stella; Milbradt, Alexander G.; Renner, Christian; Moroder, Luis

CORPORATE SOURCE: Max-Planck-Institut fuer Biochemie, Martinsried, 82152, Germany

SOURCE: Chemistry--A European Journal (2003), 9(15), 3692-3702
CODEN: CEUJED; ISSN: 0947-6539

PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA

DOCUMENT TYPE: Journal

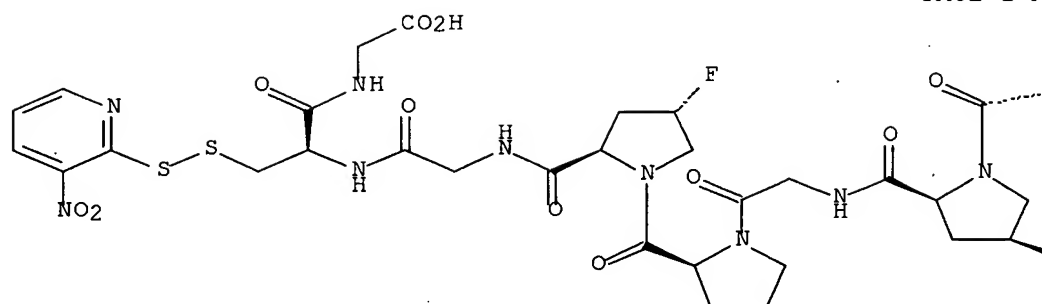
LANGUAGE: English

AB In analogy to the cystine knots present in natural collagens, a simplified disulfide cross-link was used to analyze the conformational effects of a C-terminal artificial cystine knot on the folding of collagenous peptides consisting of solely (Pro-Hyp-Gly) repeating units. Assembly of the α chains into a heterotrimer by previously applied regioselective disulfide-bridging strategies failed because of the high tendency of (Pro-Hyp-Gly)5 peptides to self-associate and form homotrimers. Only when side-chain-protected peptides were used, for example in the Hyp(tBu) form, and a new protection scheme was adopted, selective interchain-disulfide crosslinking into the heterotrimer in organic solvents was successful. This unexpected strong effect of the conformational properties on the efficiency of well-established reactions was further supported by replacing the Hyp residues with (4S)-fluoroproline, which is known to destabilize triple-helical structures. With the related [Pro-(4S)-FPro-Gly]5 peptides, assembly of the heterotrimer in aqueous solution proceeded in a satisfactory manner. Both the intermediates and the final fluorinated heterotrimer are fully unfolded in aqueous solution even at 4°. Conversely, the disulfide-crossbridged (Pro-Hyp-Gly)5 heterotrimer forms a very stable triple helix. The observation that thermal unfolding leads to scrambling of the disulfide bridges was unexpected. Although NMR expts. support an extension of the triple helix into the cystine knot, thermolysis is not associated with the unfolding process. In fact, the unstructured fluorinated trimer undergoes an equally facile thermodegrdn. associated with the intrinsic tendency of unsym. disulfides to disproportionate into sym. disulfides under favorable conditions. The exptl. results obtained with the model peptides fully support the role of triple-helix nucleation and stabilization by the artificial cystine knot as previously suggested for the natural cystine knots in collagens.

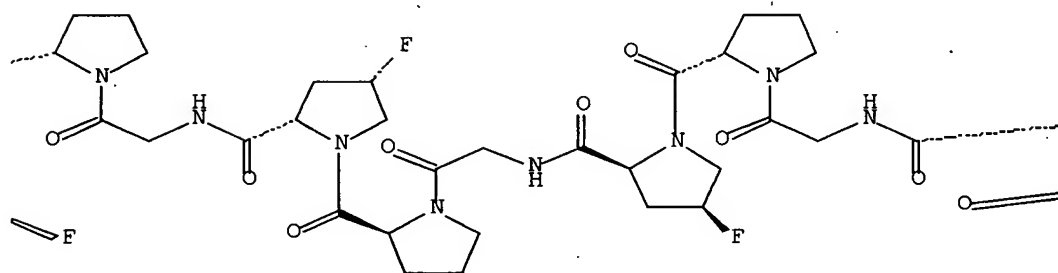
RX(37) OF 170 COMPOSED OF RX(19), RX(20)

RX(37) AU + AY ==> BD

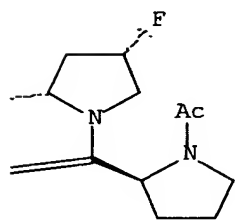
PAGE 1-A



PAGE 1-B



PAGE 1-C



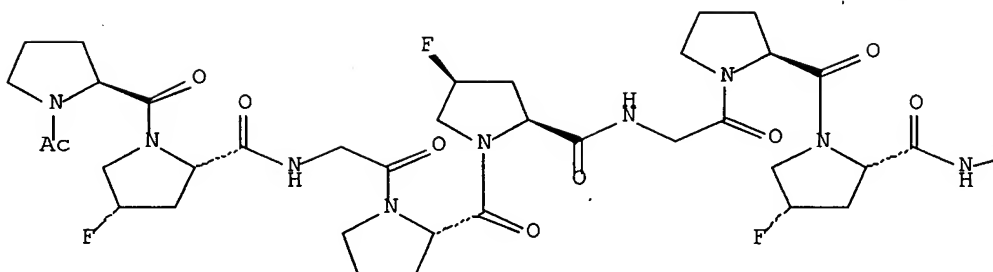
AU

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

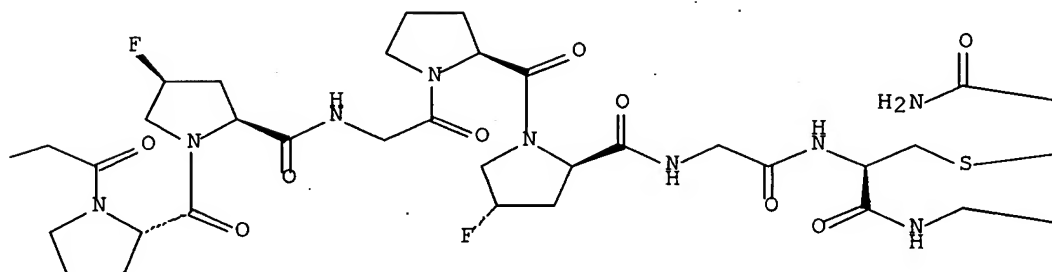
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

2
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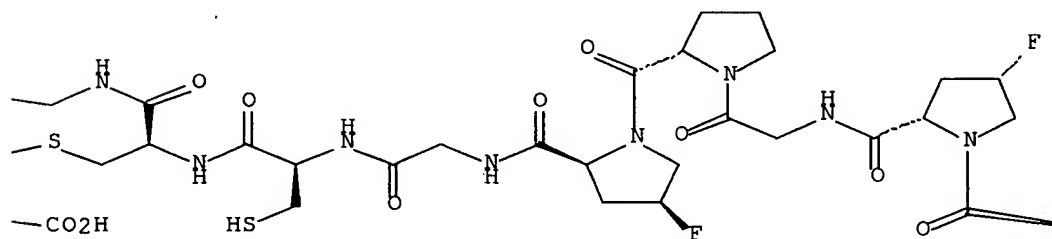
PAGE 1-A

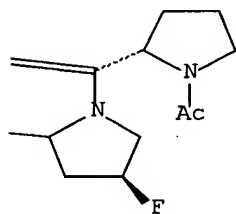
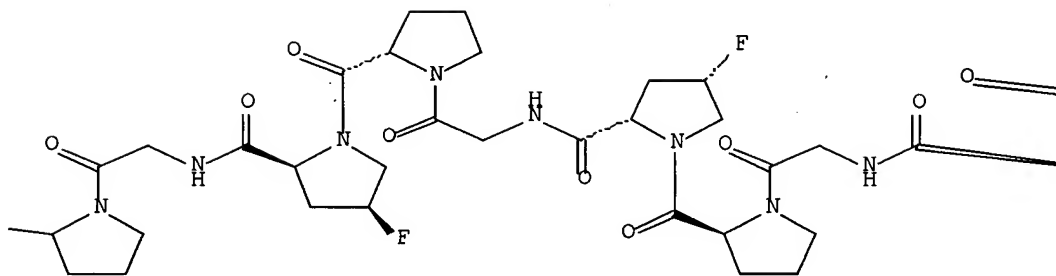


PAGE 1-B



PAGE 1-C





BD
YIELD 100%

RX(19) RCT AU **610301-61-6**, AY **610301-64-9**
 PRO BC 610301-67-2
 SOL 7732-18-5 Water
 CON 6 hours, room temperature

RX(20) RCT BC 610301-67-2
 RGT C 76-05-1 F3CCO2H, D 617-86-7 Et3SiH
 PRO BD **610301-68-3**
 SOL 7732-18-5 Water
 CON 5 minutes, room temperature

REFERENCE COUNT: 69 THERE ARE 69 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L95 ANSWER 17 OF 25 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 139:180245 CASREACT Full-text

TITLE: Synthesis of novel acceptor substrates for the dolichyl phosphate mannose synthase from yeast

AUTHOR(S): Sprung, Ines; Carmes, Laurence; Watt, Gregory M.; Flitsch, Sabine L.

CORPORATE SOURCE: School of Chemistry Centre for Protein Technology, The University of Edinburgh, Edinburgh, EH9 3JJ, UK

SOURCE: ChemBioChem (2003), 4(4), 319-332
 CODEN: CBCHFX; ISSN: 1439-4227

PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Dolichols are polyisoprenoid lipid components of mammalian membranes consisting of an average of 20 head-to-tail linked isoprene units of which the first isoprene is fully saturated. The unusual size of these lipids is intriguing and poses questions about the role of dolichol structure in biol. processes. In order to probe structure and function we have synthesized potential dolichyl analogs that retain only the first two isoprene units and carry a second functional group within the terminal lipid chain. Such analogs were evaluated as substrates for a key enzyme in the dolichyl-dependent pathway of glycan biosynthesis, dolichyl phosphate mannose (Dol-P-Man) synthase. It was shown that some functional groups, including labels such as biotin, could be tolerated. When the synthetic analogs were attached to a solid support they were still substrates for the Dol-P-Man system and thus allowed the enzymic solid-phase synthesis of glycolipids.

RX(72) OF 517 COMPOSED OF RX(34), RX(33)
 RX(72) **CM** + **CA** + 2 CE + **CF** ==>
CG + **CH**

STRUCTURE
 DIAGRAM
 IS NOT
 AVAILABLE

CM: CM 2
 reaction produ
 cts with merca
 ptopropionylam

RX(34) RCT CM 68517-67-9D

STAGE(1)

SOL 7732-18-5 Water
 CON 15 minutes, room temperature

STAGE(2)

RCT CA 503844-00-6
 SOL 64-17-5 EtOH, 7732-18-5 Water
 CON 16 hours, room temperature

STAGE(3)

RGT BB 76-05-1 F3CCO2H
 CON 10 minutes, room temperature

PRO CD 581778-62-3D

NTE solid-supported reaction, second stage is attachment to resin

RX(33) RCT CD 581778-62-3D, CE 3123-67-9

STAGE(1)

RGT CI 7786-30-3 MgCl2, CJ 1185-53-1 (HOCH2)3CNH2.HCl, CK
 9002-93-1 Ortho-Gynol
 CAT 62213-44-9 Mannosyltransferase, guanosine
 diphosphomannose-dolichol phosphate
 SOL 7732-18-5 Water

CON 21 hours, 37 deg C

STAGE(2)

RCT CF 60-24-2

SOL 7732-18-5 Water

CON 16 hours, 50 deg C

PRO CG 581778-63-4, CH 503844-07-3

NTE biotransformation, enzymic, buffered soln.

REFERENCE COUNT: 58 THERE ARE 58 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L95 ANSWER 18 OF 25 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 135:358149 CASREACT Full-text

TITLE: Improved Synthesis of C-Terminal Peptide Thioesters on
"Safety-Catch" Resins Using LiBr/THF

AUTHOR(S): Quaderer, Richard; Hilvert, Donald

CORPORATE SOURCE: Laboratory of Organic Chemistry, Swiss Federal
Institute of Technology (ETH), Zurich, CH-8092, Switz.

SOURCE: Organic Letters (2001), 3(20), 3181-3184

CODEN: ORLEF7; ISSN: 1523-7060

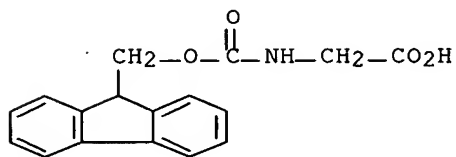
PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

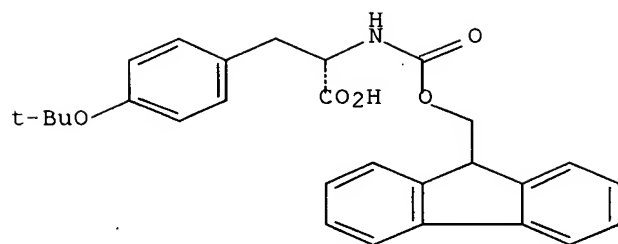
LANGUAGE: English

AB The alkanesulfonamide "safety-catch" resin has proven useful for Fmoc-based synthesis of C-terminal peptide thioesters. We now report that the yield of isolated thioester can increase significantly when the cleavage reaction is carried out in 2M LiBr/THF rather than DMF or THF. The largest effects are seen with problematic peptides that aggregate or form secondary structures on the resin.

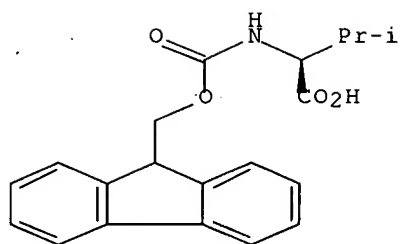
RX(2) OF 3 A + B + C + 2 D + E + F + G + 2 H + 2
N + AD ==> AE + AF



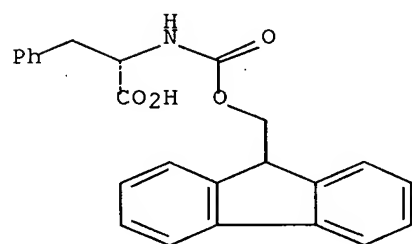
A



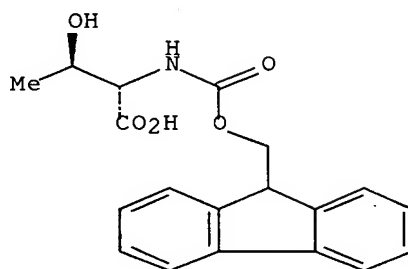
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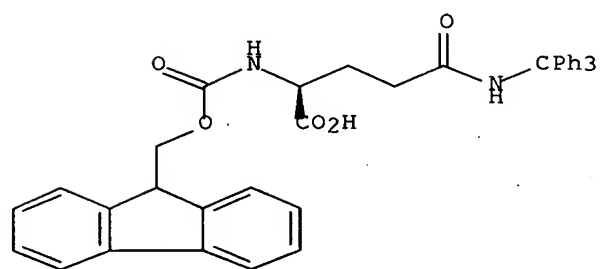
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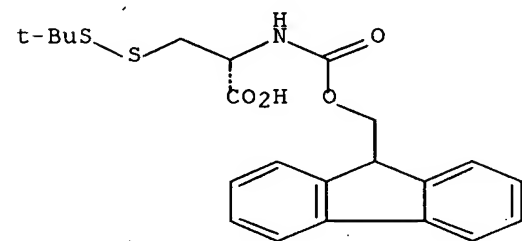
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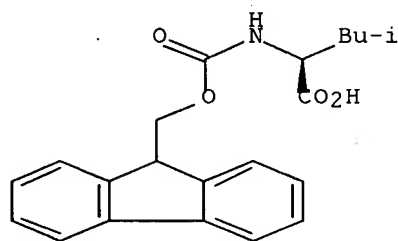
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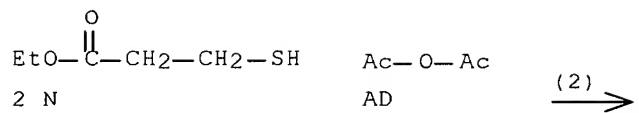
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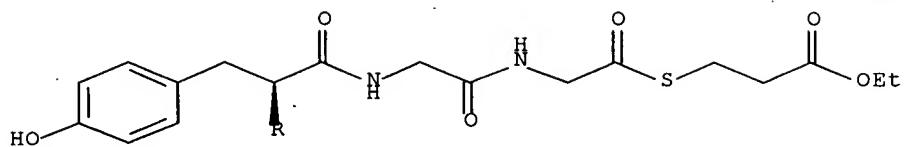
G



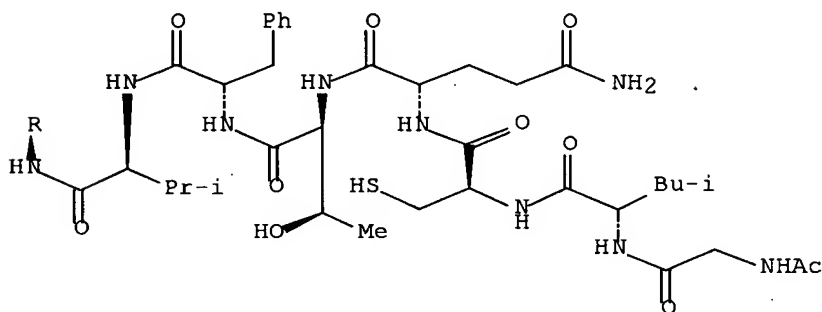
2 H



PAGE 1-A



PAGE 2-A



AE

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

—OEt



AF

RX(2) RCT A 29022-11-5

STAGE(1)

RGT P 128625-52-5 Benzotriazolol P der, Q 7087-68-5 EtN(Pr-i)2
 SOL 75-09-2 CH2Cl2

STAGE(2)

RGT R 94790-37-1 HBTU, S 2592-95-2 1-Benzotriazolol, Q
 7087-68-5 EtN(Pr-i)2
 SOL 68-12-2 DMF

STAGE(3)

RCT B 71989-38-3
 RGT R 94790-37-1 HBTU, S 2592-95-2 1-Benzotriazolol, Q
 7087-68-5 EtN(Pr-i)2
 SOL 68-12-2 DMF

STAGE(4)

RCT C 68858-20-8
 RGT R 94790-37-1 HBTU, S 2592-95-2 1-Benzotriazolol, Q
 7087-68-5 EtN(Pr-i)2
 SOL 68-12-2 DMF

STAGE(5)

RCT D 35661-40-6
 RGT R 94790-37-1 HBTU, S 2592-95-2 1-Benzotriazolol, Q
 7087-68-5 EtN(Pr-i)2
 SOL 68-12-2 DMF

STAGE(6)

RCT E 73731-37-0
 RGT R 94790-37-1 HBTU, S 2592-95-2 1-Benzotriazolol, Q

7087-68-5 EtN(Pr-i)2
SOL 68-12-2 DMF

STAGE(7)

RCT F 132327-80-1
RGT R 94790-37-1 HBTU, S 2592-95-2 1-Benzotriazolol, Q
7087-68-5 EtN(Pr-i)2
SOL 68-12-2 DMF

STAGE(8)

RCT G **73724-43-3**
RGT R 94790-37-1 HBTU, S 2592-95-2 1-Benzotriazolol, Q
7087-68-5 EtN(Pr-i)2
SOL 68-12-2 DMF

STAGE(9)

RCT H 35661-60-0
RGT R 94790-37-1 HBTU, S 2592-95-2 1-Benzotriazolol, Q
7087-68-5 EtN(Pr-i)2
SOL 68-12-2 DMF

STAGE(10)

RGT R 94790-37-1 HBTU, S 2592-95-2 1-Benzotriazolol, Q
7087-68-5 EtN(Pr-i)2
SOL 68-12-2 DMF

STAGE(11)

RGT T 24424-99-5 (Boc)2O

STAGE(12)

RGT U 18107-18-1 Me3SiCH:N2
SOL 110-54-3 Hexane, 109-99-9 THF

STAGE(13)

RCT N **5466-06-8**
RGT V 7550-35-8 LiBr
CAT 930-69-8 PhSNa
SOL 109-99-9 THF

STAGE(14)

RGT W 76-05-1 F3CCO2H, X 108-95-2 PhOH, Y 6485-79-6 Silane,
tris(1-methylethyl)-
SOL 76-05-1 F3CCO2H, 7732-18-5 Water

STAGE(15)

RCT AD 108-24-7

PRO AE **372955-83-4**, AF **372955-84-5**

NTE solid-supported reaction, first stage is attachment to
4-sulfamylbutyryl aminomethyl polystyrene (AM) resin,
alternative cleavage conditions gave lower yield, peptide
synthesis solvent assumed, 25% overall yield, piperidine
deprotection after each addn.

REFERENCE COUNT: 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L95 ANSWER 19 OF 25 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 135:115927 CASREACT Full-text

TITLE: {2Fe3S} clusters related to the di-iron sub-site of

the H-centre of all-iron hydrogenases

AUTHOR(S): Razavet, Mathieu; Davies, Sian C.; Hughes, David L.; Pickett, Christopher J.

CORPORATE SOURCE: Department of Biological Chemistry, John Innes Centre, Norwich, NR4 7UH, UK

SOURCE: Chemical Communications (Cambridge, United Kingdom) (2001), (9), 847-848
CODEN: CHCOFS; ISSN: 1359-7345

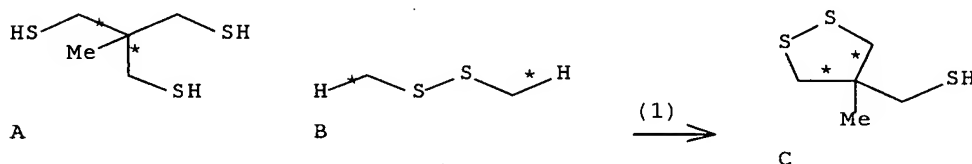
PUBLISHER: Royal Society of Chemistry

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The 1st synthetic {2Fe3S} clusters structurally related to the sub-site of the H-center of the all-iron hydrogenases, $[\text{Fe}_2(\text{CO})_5\{(\text{SCH}_2)_2\text{C}(\text{CH}_3)\text{CH}_2\text{SR}\}]$ (R = Me, CH_2Ph), are prepared and characterized by x-ray crystallog. In the complexes tripodal dithiolate thioether ligands gave di-iron pentacarbonyls with differential (2:3) S-ligation of the Fe atoms.

RX(1) OF 20 **A + B ==> C...**



RX(1) RCT A 39597-87-0, B 624-92-0
 PRO C 110206-42-3

REFERENCE COUNT: 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L95 ANSWER 20 OF 25 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 134:237823 CASREACT Full-text

TITLE: Synthesis and conformational analysis of the insulin-like 4 gene product

AUTHOR(S): Bullesbach, Erika E.; Schwabe, C.

CORPORATE SOURCE: Department of Biochemistry and Molecular Biology, Medical University of South Carolina, Charleston, SC, 29425, USA

SOURCE: Journal of Peptide Research (2001), 57(1), 77-83

CODEN: JPERFA; ISSN: 1397-002X

PUBLISHER: Munksgaard International Publishers Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

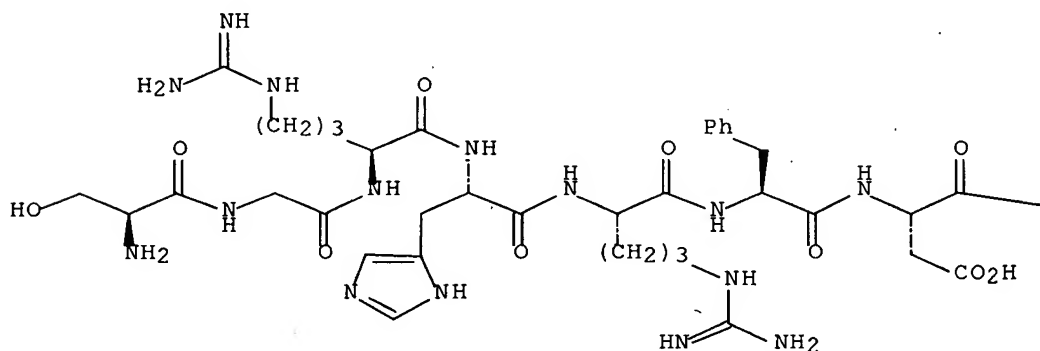
AB Insulin-like 4 (INSL-4) is a protein expressed in the early placenta. Its primary structure is insulin-like with reference to the distribution of cysteine residues and the single chain pro-form. Insulin-like 4 was generated by solid-phase peptide synthesis of the two chains followed by the sequential synthesis of the three disulfide bonds. Two disulfide isomers were produced, one with an insulin-like disulfide bonding pattern and the other with a reversed chain orientation. The CD spectra of the two disulfide isomers were

indistinguishable without any features produced by periodic structures. In addition, the hydrodynamic properties of the two isomers were identical which implied a very open structure of the disulfide-bonded two-chain mols. It appears that insulin-likeness cannot be defined solely on the basis of the primary structure of cDNA.

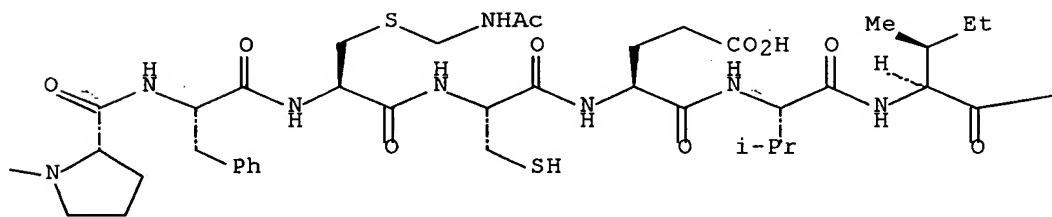
RX(3) OF 3 COMPOSED OF RX(1), RX(2)

RX(3) **A** + **M** ==> **N**

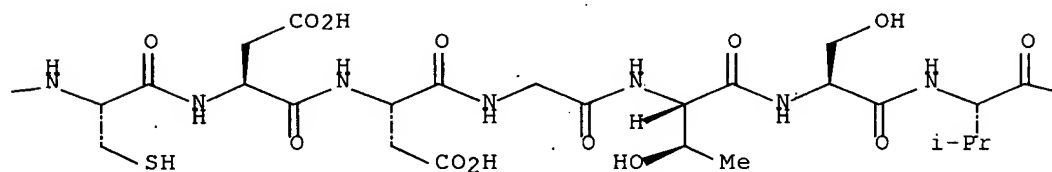
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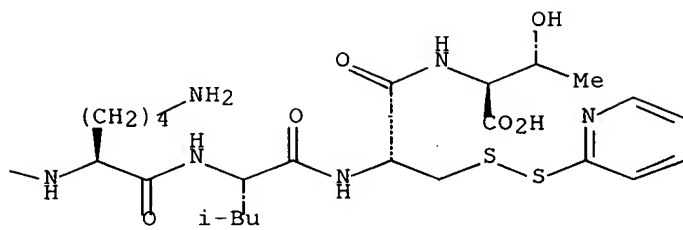
PAGE 1-B



PAGE 1-C



PAGE 1-D



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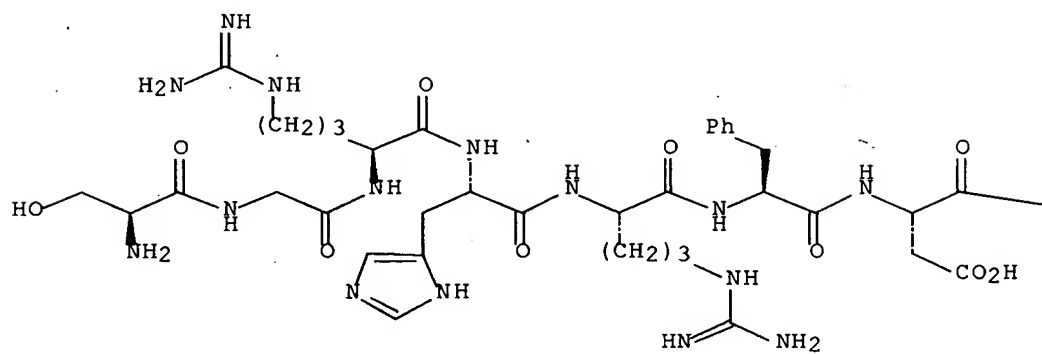
M

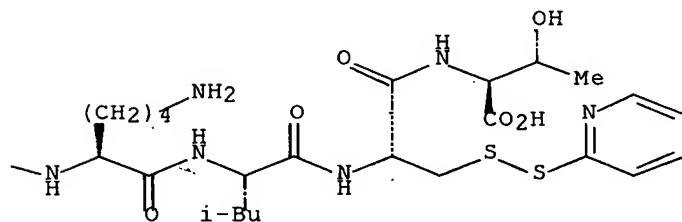
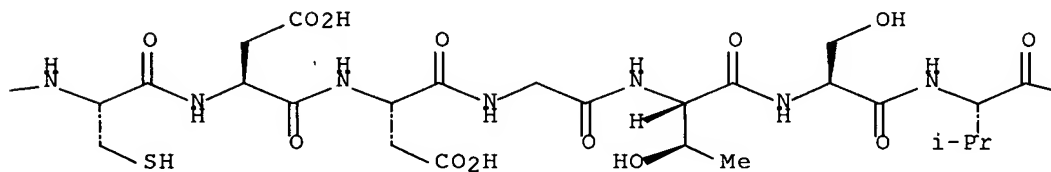
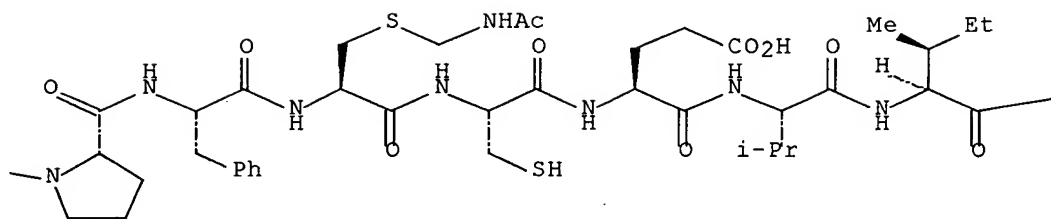
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AVAILABLE

N: CM 1

PAGE 1-A





N: CM 2

RX(1) RCT A 330548-24-8

STAGE(1)

SOL 64-19-7 AcOH

STAGE(2)

RGT C 7553-56-2 I2

SOL 64-19-7 AcOH

STAGE(3)

RGT D 50-81-7 (L)-Ascorbic acid

SOL 7732-18-5 Water

STAGE(4)

RGT E 2127-03-9 2-Pyridyl disulfide, F 100-68-5 PhSMe
SOL 76-05-1 F3CCO2H

STAGE(5)

RGT G 1493-13-6 F3CSO2H
SOL 76-05-1 F3CCO2H

STAGE(6)

RGT H 631-61-8 NH4OAc
SOL 75-05-8 MeCN

PRO B 209249-20-7
NTE stereoselective

RX(2) RCT B 209249-20-7, M 330625-42-8

STAGE(1)

RGT O 1066-33-7 NH4 bicarbonate
SOL 7732-18-5 Water

STAGE(2)

RGT I 64-19-7 AcOH

PRO N **330637-72-4**
NTE stereoselective

REFERENCE COUNT: 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L95 ANSWER 21 OF 25 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 132:49741 CASREACT Full-text

TITLE: Synthesis and mass spectral characterization of
diisopropylamino-ethanethiol, -sulfides and
-disulfides and vinyl sulfides

AUTHOR(S): Rohrbach, D. K.; Berg, F. J.; Szafraniec, L. J.;
Rossman, D. I.; Durst, H. D.; Munavalli, S.

CORPORATE SOURCE: Edgewood Research Development and Engineering Center,
Aberdeen Proving Ground, U.S. Army, Aberdeen, MD,
21010, USA

SOURCE: Phosphorus, Sulfur and Silicon and the Related
Elements (1999), 149, 95-106
CODEN: PSSLEC; ISSN: 1042-6507

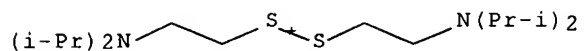
PUBLISHER: Gordon & Breach Science Publishers

DOCUMENT TYPE: Journal

LANGUAGE: English

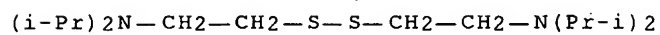
AB The sulfur containing chemical agent, O-ethyl-S-2-
(diisopropylaminoethyl)methylphosphonothiolate, is an extremely potent
inhibitor of the enzyme acetylcholinesterase and exhibits extended neurol.
effects. It undergoes degradation on standing alone or in the environment.
Hence, identification of its primary degradation products assumes considerable
importance. The synthesis and mass spectral fragmentation behavior of the
title compds., some of which are present in the O-ethyl-S-2-
(diisopropylaminoethyl)methyl phosphonothiolate degradation products, has not
received much attention. This communication describes the synthesis and mass
spectral characterization of the title compds.

RX(2) OF 2 3 G + H ==> I + J
+ K



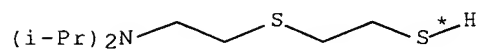
● 2 HCl

2 G



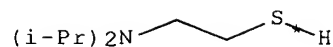
● 2 HCl

G

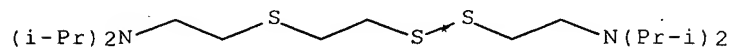


H

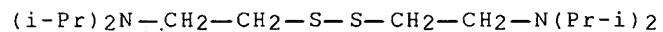
(2) →



I
YIELD 24%



J
YIELD 27%



K
YIELD 31%

RX(2) RCT G 252963-82-9

STAGE(1)

RGT L 7791-25-5 SO2Cl2

SOL 75-09-2 CH2Cl2

STAGE(2)

RCT H 168885-96-9
SOL 75-09-2 CH2Cl2

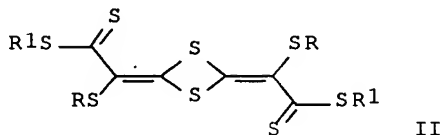
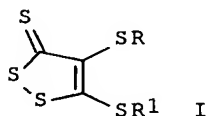
STAGE(3)

RGT M 1310-73-2 NaOH
SOL 7732-18-5 Water

PRO I 5842-07-9, J 110501-59-2, K
65332-44-7

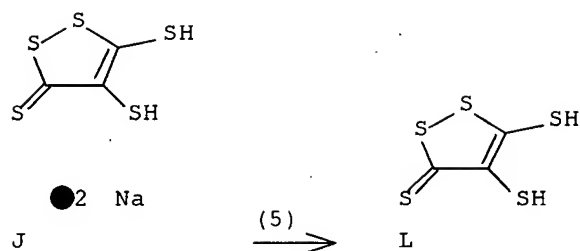
REFERENCE COUNT: 44 THERE ARE 44 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L95 ANSWER 22 OF 25 CASREACT. COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 129:189320 CASREACT Full-text
TITLE: Synthesis and stereochemistry of bis(dithiacrown
ether)- and dodecylthio-substituted (E)-thiodesaurines
AUTHOR(S): Rudershausen, Sandra; Drexler, Hans-Joachim; Holdt,
Hans-Juergen
CORPORATE SOURCE: Fachbereich Chemie, Universitaet Rostock, Rostock,
D-18051, Germany
SOURCE: Journal fuer Praktische Chemie/Chemiker-Zeitung
(1998), 340(5), 450-454
CODEN: JPCCEM; ISSN: 0941-1216
PUBLISHER: Johann Ambrosius Barth
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



AB Reductive dimerization of 1,2-dithiole-3-thiones I [R = dodecyl, R1 = Me; R, R1 = dodecyl; RR1 = CH2(CH2OCH2)nCH2, n = 2-4] with P(OEt)3 furnished the corresponding thiodesaurines II. The stereochem. of II [RR1 = CH2(CH2OCH2)nCH2, n = 3] was determined by x-ray crystallog. anal.

RX(5) OF 17 J ==> L...



RX(5) RCT J **100890-76-4**
 RGT M 7647-01-0 HCl
 PRO L **69995-95-5**
 SOL 7732-18-5 Water

L95 ANSWER 23 OF 25 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 125:47583 CASREACT [Full-text](#)

TITLE: N10-(2'-Mercaptoethanoyl)-2,2,5,5-tetramethyl-3,4-dithia-7,10-diazabicyclo[5.3.0]decane and its reaction with oxotrichlorobis(triphenylphosphine)rhenium(V)

AUTHOR(S): Alarabi, H.; Bell, R. A.; Howard-Lock, H. E.; Kowanetz, J.; Lock, C. J. L.

CORPORATE SOURCE: Lab. Inorganic Med., McMaster Univ., Hamilton, ON, L8S 4M1, Can.

SOURCE: Canadian Journal of Chemistry (1996), 74(4), 574-582
 CODEN: CJCHAG; ISSN: 0008-4042

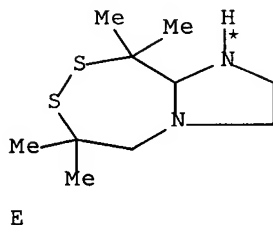
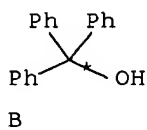
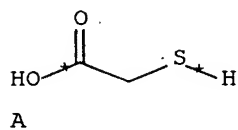
PUBLISHER: National Research Council of Canada

DOCUMENT TYPE: Journal

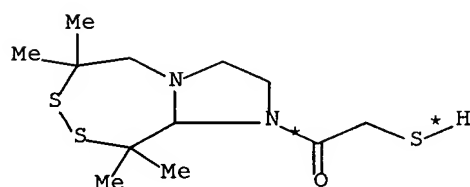
LANGUAGE: English

AB The ligand mol. N10-(2'-mercaptoethanoyl)-2,2,5,5-tetramethyl-3,4-dithia-7,10-diazabicyclo[5.3.0]decane was prepared and characterized by ¹H and ¹³C NMR spectroscopy and by mass spectrometry. The protected analog, N10-[(2'-triphenylmethylthio)ethanoyl]-2,2,5,5-tetramethyl-3,4-dithia-7,10-diazabicyclo[5.3.0]decane dimethanol hemihydrate, was examined by the same techniques and also by x-ray crystallog. Crystals were triclinic, P₁h1v1n1, a 11.125(2), b 11.986(2), c 13.562(3) Å, α 103.54(3), β 90.29(3), γ 107.11(3)°, and Z = 2. The crystal was unstable in air at room temperature, so measurements were made on a crystal sealed in a tube that contained MeOH vapor. The structure was solved by direct methods and refined to R = 0.1497, Rw = 0.0655 based on 5000 independent reflections. The high residuals were caused by solvent disorder. Bond lengths and angles were normal. The reaction of the ligand with ReOCl₃(PPh₃)₂ yielded an unexpected asym. complex, oxo(1,1-dimethyl-1,8-dimercapto-3,6-diazaoctan-7-onato- N3,N6,S1,S8)rhenium. Crystals were monoclinic, space group P2₁/n, a 10.633(2), b 11.221(2), c 11.678(1) Å, β 116.10(1)°, Z = 4. The structure was solved by the heavy atom method and refined to R = 0.0471, Rw = 0.0340 based on 2866 unique reflections. Most bond lengths and angles were normal. The Re-tp1bond.O distance of 1.681(5) Å was longer than normal. It is postulated that this was caused by competitive π bonding between the deprotonated amidic N atom and the Re atom, as shown by the short Re-N distance (1.997(6) Å) compared to the equivalent distance for the amine N atom (Re-N, 2.151(4) Å).

RX(6) OF 6 COMPOSED OF RX(1), RX(2), RX(3)

RX(6) **A** + **B** + **E** ==> **I**

3
STEPS
→



YIELD 75%

RX(1) RCT A **68-11-1**, B 76-84-6
 RGT D 64-19-7 AcOH
 PRO C 34914-36-8
 NTE 20-70.deg.

RX(2) RCT C 34914-36-8, E **108168-04-3**
 RGT G 538-75-0 DCC
 PRO F 178113-10-5
 SOL 75-09-2 CH2Cl2

RX(3) RCT F 178113-10-5
 RGT J 76-05-1 F3CCO2H, K 617-86-7 Et3SiH
 PRO I **178113-13-8**
 NTE 20.deg.

L95 ANSWER 24 OF 25 CASREACT COPYRIGHT 2007 ACS on STN

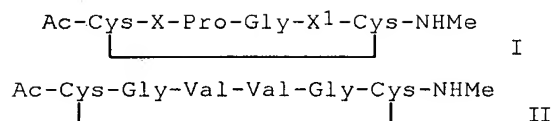
ACCESSION NUMBER: 109:190804 CASREACT Full-text

TITLE: Chain reversals in model peptides: studies of
 cystine-containing cyclic peptides. II. Effects of
 valyl residues and possible i-to-(i + 3) attractive
 ionic interactions on cyclization of [Cys1],[Cys6]
 hexapeptides

AUTHOR(S): Milburn, P. J.; Meinwald, Y. C.; Takahashi, S.; Oi,
 T.; Scheraga, H. A.

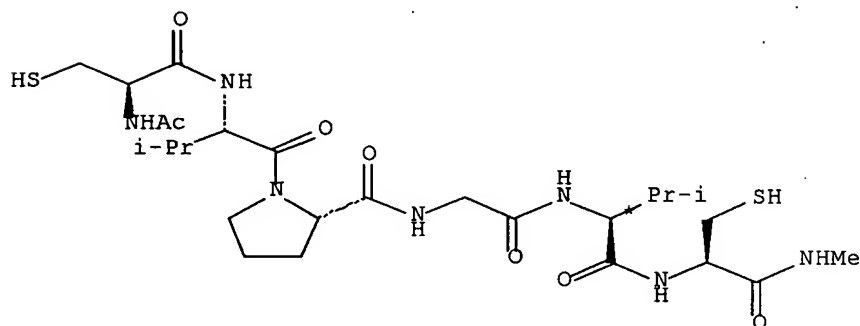
CORPORATE SOURCE: Baker Lab. Chem., Cornell Univ., Ithaca, NY,
 14853-1301, USA

SOURCE: International Journal of Peptide & Protein Research

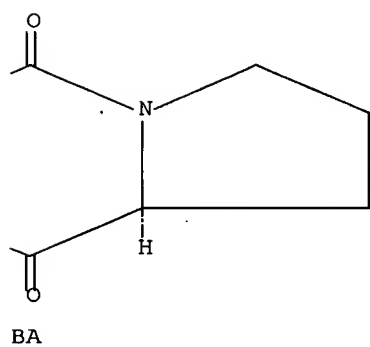
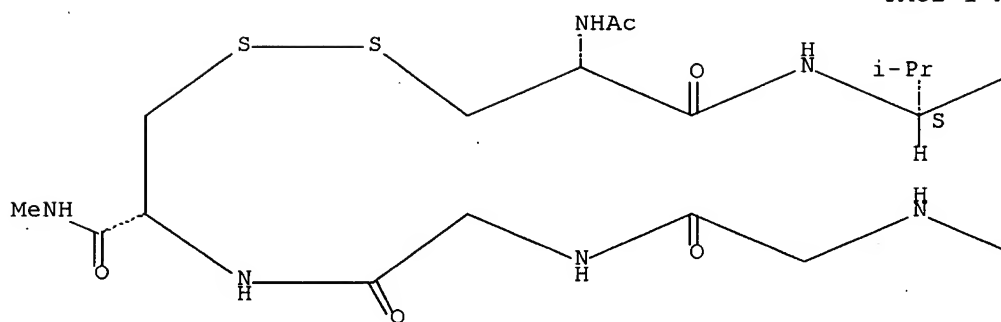


AB The synthesis of cystine-containing hexapeptides I (X = Glu, X¹ = Lys; X = Lys, X¹ = Glu; X = X¹ = Val) and II is described. These were used in disulfide-exchange reactions with peptide I (X = Val, X¹ = Gly) as the formal oxidant. The relative propensities for peptide cyclization were thus deduced, and the tendency toward the formation of chain-reversal conformations was established. quant. Ac-Cys-(Val)₄-Lys-NHMe was prepared but was never obtained as the cyclic monomer, demonstrating that the formation of chain-reversals in this peptide was of very low probability. Incorporation of pairs of valyl residues decreased the ease of cyclization, but conformational flexibility in the cystine-containing hexapeptides may have compensated for substitutions which hinder the adoption of certain β -turn conformations. The peptides containing ionic residues were cyclized more readily than expected, and this process was relatively insensitive to salt concentration. This observation is discussed with regard to the stabilization of β -turns by i to $(i + 3)$ ionic interactions in peptides and proteins. A method for blocking thiols was introduced as an important in the anal. of the equilibrium mixts.

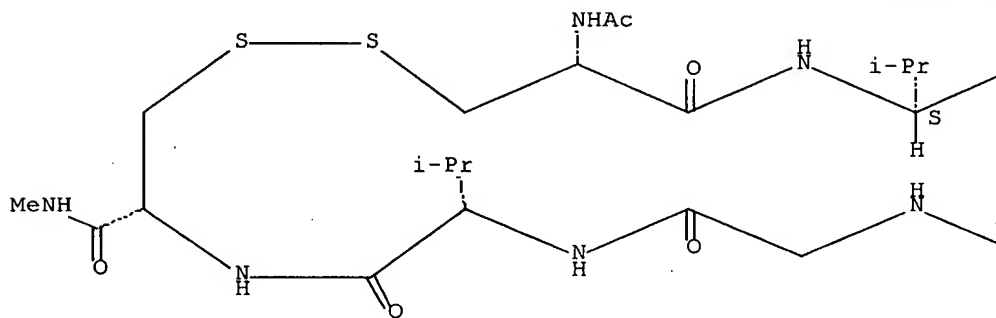
RX(35) OF 210 **AY** + **BA** ==> **AR** + **BB**

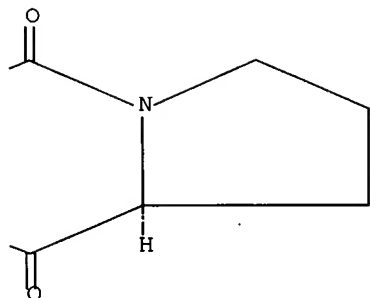


AY

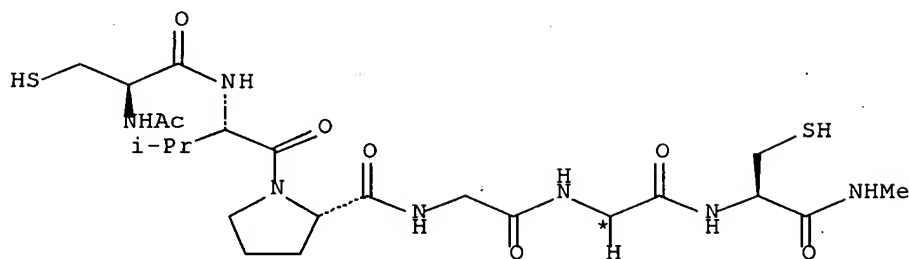


(35) →





AR



BB

RX(35) RCT AY 117049-00-0, BA 108594-51-0
 PRO AR 117048-95-0, BB 117049-02-2
 NTE equil., pH 8.0 buffer

L95 ANSWER 25 OF 25 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 103:6696 CASREACT Full-text

TITLE: A nuclear magnetic resonance study of the formation and conformational equilibria of symmetrical and mixed disulfides of captopril

AUTHOR(S): Rabenstein, Dallas L.; Theriault, Yvon

CORPORATE SOURCE: Dep. Chem., Univ. Alberta, Edmonton, AB, T6G 2G2, Can.

SOURCE: Canadian Journal of Chemistry (1985), 63(1), 33-9

CODEN: CJCHAG; ISSN: 0008-4042

DOCUMENT TYPE: Journal

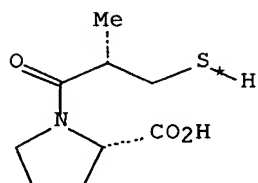
LANGUAGE: English

AB The oxidation of captopril (CpSH) [1-(D-3-mercapto-2-methylpropanoyl)-L-proline] by glutathione disulfide (GSSG) via thiol/disulfide exchange to form, in the first step, CpSSG and GSH and, in the second step, CpSSCp and GSH, has been studied in aqueous solution by 1H NMR. Due to slow rotation around the amide bond(s) of CpSH and CpSSCp and of the captopril part of CpSSG, sep. resonances are observed for the cis and trans conformations across these bonds. Conformational equilibrium consts. were estimated as a function of pH for CpSH, CpSSCp, and CpSSG from the intensities of resonances for the cis and

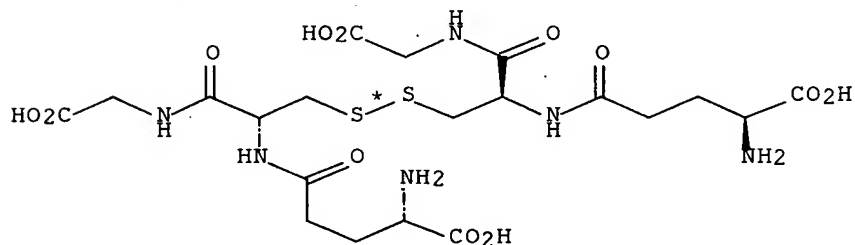
trans isomers. These equilibrium consts. were used in the determination of equilibrium consts. for the two steps in the oxidation of CpSH by GSSG. CpSH has a greater tendency to reduce disulfide bonds by thiol/disulfide exchange at physiol. pH, and thus form mixed disulfides, than do the thiol groups in amino acids. Also, the conformational equilibrium constant indicate that, at phys. pH, approx. two thirds of the captopril, either free or in a disulfide form has the trans conformation.

RX(1) OF 3 **A** + 2 **B** ==> **C** + **D**

...

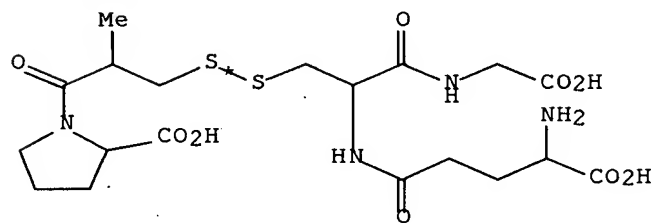


A

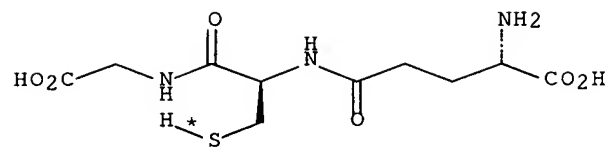


2 **B**

(1) →



C



D

RX(1) RCT A **62571-86-2**, B **27025-41-8**
RGT E 7447-40-7 KCl, F 75-65-0 t-BuOH, G 139-33-3 Di-Na EDTA
PRO C **78636-30-3**, D **70-18-8**
SOL 7789-20-0 D2O

=> d his full

(FILE 'HOME' ENTERED AT 13:46:45 ON 28 SEP 2007)

FILE 'ZCAPLUS' ENTERED AT 13:46:57 ON 28 SEP 2007

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      E US2007-569710/APPS
L*** DEL      1 S US2007-569710/AP
              D SCA
              E US2006-569710/APPS
              E WO2004-2774/APPS
              E WO2004-IB2774/APPS
L2            1 SEA ABB=ON  PLU=ON  WO2004-IB2774/AP
              SEL RN
              D IALL L2

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              D SCA
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              D SCA
L5            1 SEA ABB=ON  PLU=ON  709044-44-0
              D SCA
L6            1 SEA ABB=ON  PLU=ON  847493-45-2
              D SCA
L7            1 SEA ABB=ON  PLU=ON  70-18-8
              D SCA
L8            1 SEA ABB=ON  PLU=ON  6088-50-2
              D SCA
L9            1 SEA ABB=ON  PLU=ON  105988-28-1
              D SCA
L10           1 SEA ABB=ON  PLU=ON  847493-44-1
              D SCA
L11           1 SEA ABB=ON  PLU=ON  847493-46-3
              D SCA

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FILE 'ZCAPLUS' ENTERED AT 13:57:44 ON 28 SEP 2007

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L12           9 SEA ABB=ON  PLU=ON  L8 OR L10
              D SCA
              E THIOLS+ALL/CT
L13           26734 SEA ABB=ON  PLU=ON  THIOLS+OLD/CT
L14           264757 SEA ABB=ON  PLU=ON  PUR/RL
L15           32 SEA ABB=ON  PLU=ON  L13 (L) L14
              E DISULFIDES+ALL/CT
L16           118162 SEA ABB=ON  PLU=ON  DISULFID?/BI
L17           147 SEA ABB=ON  PLU=ON  DI SULFID?/BI
L18           1626 SEA ABB=ON  PLU=ON  BISULFID?/BI OR BI SULFID?/BI
L19           11 SEA ABB=ON  PLU=ON  L15 AND (L16 OR L17 OR L18)
              D SCA
              E DISULFIDES+ALL/CT
L20           3625 SEA ABB=ON  PLU=ON  DISULFIDES/CT
L21           7 SEA ABB=ON  PLU=ON  L20 (L) L14
L22           167140 SEA ABB=ON  PLU=ON  ?THIOL?/BI
L23           1 SEA ABB=ON  PLU=ON  L21 AND L22
              D SCA
L24           120255 SEA ABB=ON  PLU=ON  ?DISULFID?/BI
L25           167140 SEA ABB=ON  PLU=ON  ?THIOL?/BI
L26           20268 SEA ABB=ON  PLU=ON  L24 AND L25

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10/569710

| | | | | |
|-----|---------|---------------------|--------|--|
| L27 | 856378 | SEA ABB=ON | PLU=ON | ?PURIF?/BI |
| L28 | 1351 | SEA ABB=ON | PLU=ON | L26 AND L27 |
| L29 | 97550 | SEA ABB=ON | PLU=ON | ?GLUTATHION?/BI |
| L30 | 253 | SEA ABB=ON | PLU=ON | L28 AND L29 |
| L31 | 14 | SEA ABB=ON | PLU=ON | (L3 OR L5 OR L6 OR (L8 OR L9 OR L10 OR L11)) AND L26 |
| | | D SCA | | |
| L32 | 4 | SEA ABB=ON | PLU=ON | L19 AND 75-15-0?/OBI |
| | | D SCA | | |
| L33 | 7 | SEA ABB=ON | PLU=ON | L19 NOT L32 |
| | | D SCA | | |
| L34 | 7 | SEA ABB=ON | PLU=ON | L21 NOT L33 |
| | | D SCA | | |
| | | D SCA L21 | | |
| | | E MERCAPTANS+ALL/CT | | |
| | | D SCA L31 | | |
| L35 | 2 | SEA ABB=ON | PLU=ON | L31 AND ?ISOLAT?/OBI |
| L36 | 1 | SEA ABB=ON | PLU=ON | L31 AND TOTAL/TI |
| L37 | 1 | SEA ABB=ON | PLU=ON | L31 AND REDUCTION?/TI |
| L38 | 10 | SEA ABB=ON | PLU=ON | L33 OR L35 OR L36 OR L37 |
| | | D SCA | | |
| | | D COST | | |
| L39 | 166847 | SEA ABB=ON | PLU=ON | ?MERCAPT?/BI |
| L40 | 99071 | SEA ABB=ON | PLU=ON | ?THIOL?/AB |
| L41 | 97340 | SEA ABB=ON | PLU=ON | ?MERCAPT?/AB |
| L42 | 68341 | SEA ABB=ON | PLU=ON | ?DISULFID?/AB |
| L43 | 618440 | SEA ABB=ON | PLU=ON | ?PURIF?/AB |
| L44 | 1062429 | SEA ABB=ON | PLU=ON | ?ISOLAT?/AB |
| L45 | 2544 | SEA ABB=ON | PLU=ON | (L41 OR L40) AND L42 AND (L43 OR L44) |
| L46 | 195 | SEA ABB=ON | PLU=ON | L14 AND L45 |
| | | D KWIC 1 | | |
| | | D KWIC 50 | | |
| L47 | 65 | SEA ABB=ON | PLU=ON | L3 |
| L48 | 1 | SEA ABB=ON | PLU=ON | L46 AND L47 |
| | | D SCA | | |
| L49 | 1 | SEA ABB=ON | PLU=ON | L8 AND L46 |
| L50 | 1 | SEA ABB=ON | PLU=ON | L9 AND L46 |
| L51 | 19 | SEA ABB=ON | PLU=ON | (L8 OR L9 OR L10) |
| L52 | 10 | SEA ABB=ON | PLU=ON | L33 OR (L35 OR L36 OR L37) |
| L53 | 16 | SEA ABB=ON | PLU=ON | L51 NOT L52 |
| | | D SCA | | |
| | | E STEENCAMP D/AU | | |
| | | E STEINCAMP D/AU | | |
| | | D AU L2 | | |
| | | E STEENKAMP D/AU | | |
| L54 | 60 | SEA ABB=ON | PLU=ON | STEENKAMP D?/AU |
| L55 | 2 | SEA ABB=ON | PLU=ON | L52 AND L54 |
| | | D SCA | | |
| L56 | 3 | SEA ABB=ON | PLU=ON | L28 AND L54 |
| L57 | 1 | SEA ABB=ON | PLU=ON | L56 NOT L55 |
| | | D SCA | | |
| | | D SCA L23 | | |
| L58 | 3 | SEA ABB=ON | PLU=ON | L39 AND L21 |
| | | D SCA | | |
| L59 | 2 | SEA ABB=ON | PLU=ON | L5 |
| L60 | 1 | SEA ABB=ON | PLU=ON | L6 |
| L61 | 1 | SEA ABB=ON | PLU=ON | L11 |
| L62 | 2 | SEA ABB=ON | PLU=ON | (L59 OR L60 OR L61) |
| | | D SCA | | |
| L63 | 9 | SEA ABB=ON | PLU=ON | L8 |

L64 1 SEA ABB=ON PLU=ON L10
 L65 9 SEA ABB=ON PLU=ON (L63 OR L64)
 D SCA
 L66 6 SEA ABB=ON PLU=ON L65 AND MERCAPTO?/OBI
 L67 6 SEA ABB=ON PLU=ON L65 AND MERCAPTO/OBI
 L68 15061 SEA ABB=ON PLU=ON MERCAPTO GROUP/CT
 L69 1 SEA ABB=ON PLU=ON L65 AND L68
 L70 2 SEA ABB=ON PLU=ON L3 AND L45
 D SCA
 L71 2 SEA ABB=ON PLU=ON L3/PUR
 D SCA
 L72 993 SEA ABB=ON PLU=ON L20 (L) (RGT OR RCT OR RACT)/RL
 L73 1831 SEA ABB=ON PLU=ON L13 (L) (PRU OR PREP)/RL
 L74 32 SEA ABB=ON PLU=ON L13 (L) (PUR)/RL
 L75 46 SEA ABB=ON PLU=ON L72 AND (L73 OR L74)
 L76 1 SEA ABB=ON PLU=ON L74 AND L72
 D SCA
 L77 0 SEA ABB=ON PLU=ON L21 AND L73
 L78 0 SEA ABB=ON PLU=ON L21 AND L74
 L79 1355 SEA ABB=ON PLU=ON L13 AND L20
 L80 56 SEA ABB=ON PLU=ON L79 AND L45
 L81 424326 SEA ABB=ON PLU=ON PURIF?/OBI
 L82 287765 SEA ABB=ON PLU=ON ISOLAT?/OBI
 L83 2 SEA ABB=ON PLU=ON L80 AND L81
 L84 1 SEA ABB=ON PLU=ON L80 AND L82
 L85 3 SEA ABB=ON PLU=ON (L83 OR L84)
 D SCA

FILE 'CASREACT' ENTERED AT 16:32:54 ON 28 SEP 2007

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 E THI/FG.RCT
 E DISU/FG.PRO
 L86 1384 SEA ABB=ON PLU=ON THIOL/FG.RCT (L) DISULFIDE/FG.PRO
 E DISULFIDE/FG.RCT
 L87 505 SEA ABB=ON PLU=ON DISULFIDE/FG.RCT (L) THIOL/FG.PRO
 L88 123 SEA ABB=ON PLU=ON L86 AND L87
 L89 12 SEA ABB=ON PLU=ON L86 (L) L87
 D SCA

FILE 'CAPLUS' ENTERED AT 16:38:03 ON 28 SEP 2007

L90 12 SEA ABB=ON PLU=ON L89
 D SCA
 L91 123 SEA ABB=ON PLU=ON L88
 L92 11 SEA ABB=ON PLU=ON (L43 OR L44) AND L91
 D SCA

FILE 'REGISTRY' ENTERED AT 16:40:52 ON 28 SEP 2007

FILE 'ZCAPLUS' ENTERED AT 16:40:57 ON 28 SEP 2007

 D STAT QUE L55
 D STAT QUE L56
 L93 3 SEA ABB=ON PLU=ON L55 OR L56
 D IBIB ABS HITIND HITSTR L93 1-3

FILE 'REGISTRY' ENTERED AT 16:41:51 ON 28 SEP 2007

FILE 'ZCAPLUS' ENTERED AT 16:41:54 ON 28 SEP 2007

 D STAT QUE L33
 D STAT QUE L35
 D STAT QUE L36

D STAT QUE L37
 D STAT QUE L23
 D STAT QUE L58
 D STAT QUE L62
 D STAT QUE L69
 D STAT QUE L71

L94 13 SEA ABB=ON PLU=ON (L33 OR L35 OR L36 OR L37 OR L23 OR L58 OR
 L62 OR L69 OR L71) NOT (L55 OR L56)

FILE 'CASREACT' ENTERED AT 16:43:08 ON 28 SEP 2007
 D STAT QUE L89

L95 FILE 'ZCAPLUS, CASREACT' ENTERED AT 16:43:37 ON 28 SEP 2007
 25 DUP REM L94 L89 (0 DUPLICATES REMOVED)
 ANSWERS '1-13' FROM FILE ZCAPLUS
 ANSWERS '14-25' FROM FILE CASREACT
 D IBIB ABS HITIND HITSTR L95 1-13
 D IBIB ABS FHIT L95 14-25

FILE 'ZCAPLUS' ENTERED AT 16:46:11 ON 28 SEP 2007

FILE 'ZCAPLUS, CASREACT' ENTERED AT 16:46:16 ON 28 SEP 2007
 D IBIB ABS FHIT L95 14-25

FILE HOME

FILE ZCAPLUS

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FILE COVERS 1907 - 28 Sep 2007 VOL 147 ISS 15
 FILE LAST UPDATED: 27 Sep 2007 (20070927/ED)

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FILE REGISTRY

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 27 SEP 2007 HIGHEST RN 948530-59-4
 DICTIONARY FILE UPDATES: 27 SEP 2007 HIGHEST RN 948530-59-4

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FILE CASREACT

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FILE CONTENT:1840 - 22 Sep 2007 VOL 147 ISS 14

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*****
*
*      CASREACT now has more than 12 million reactions
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FILE CAPLUS

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